Technical Report IRRP-97-4
August 1997

US Army Corps of Engineers
Waterways Experiment Station

Installation Restoration Research Program

Documentation on Limitations and Applicabilities of the Use of Off-the-Shelf Groundwater Models in Site Cleanup

by *Carlos E. Ruiz, Mansour Zakikhani, Christian J. McGrath, Patrick N. Deliman, Stacy Howington, Robert A. Evans, Fred T. Tracy*

Prepared for Headquarters, U.S. Army Corps of Engineers

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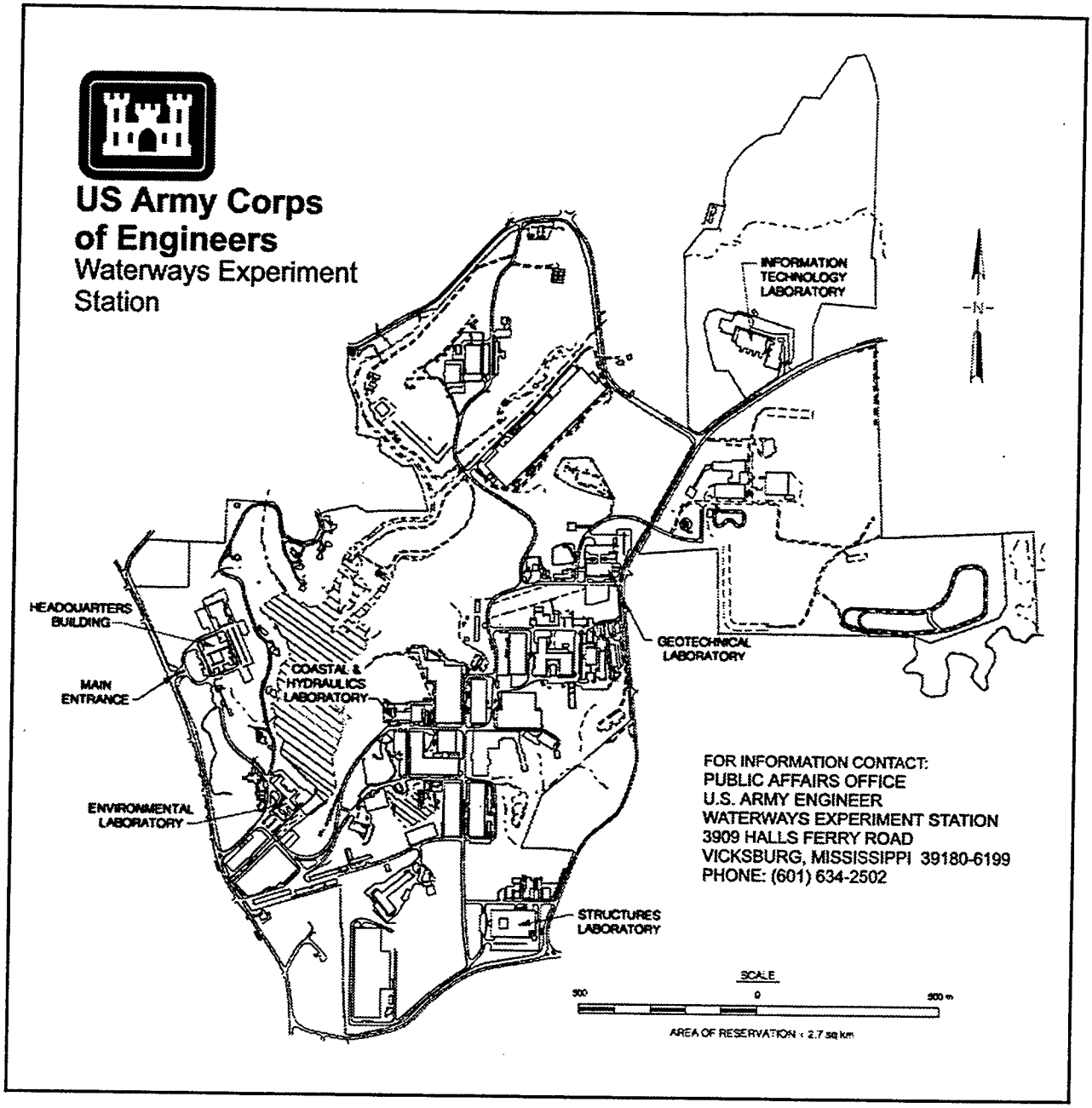

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Preface

The work reported herein was conducted by the Environmental Laboratory (EL), the Coastal and Hydraulics Laboratory (CHL), and the Information Technology Laboratory (ITL) of the U.S. Army Engineer Waterways Experiment Station (WES), Vicksburg, MS. The research was sponsored by the Department of Army Installation Restoration Research Program (IRRP), Environmental Quality and Technology, Work Unit entitled "Groundwater Model Assessment," Project No. AF25-GW-001.
Dr. Clem Myer was the IRRP Coordinator at the Directorate of Research and Development, Headquarters, U.S. Army Corps of Engineers (HQUSACE). Dr. Bob York of the U.S. Army Environmental Center and Mr. Jim Baliff of the Environmental Restoration Division, Directorate of Military Programs, HQUSACE, served as the IRRP Overview Committee. Mr. Ira May and Ms. Tomiann McDaniel were Technical Monitors for the IRRP. Dr. Jeffery P. Holland, WES, was the Groundwater Modeling Program Manager. Dr. M. John Cullinane, WES, was the IRRP Program Manager.

The study was conducted by Drs. Carlos E. Ruiz, Mansour Zakikhani, and Patrick N. Deliman and Mr. Christian J. McGrath of the Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED), EL; Mr. Stacy Howington of the Reservoir Water Quality Branch and Mr. Robert A. Evans of the Estuarine Simulation Branch, Estuaries Division, CHL; and Dr. Fred T. Tracy of the Interdisciplinary Research Group (IRG), Computer-Aided Engineering Division (CAED), ITL.

The study was conducted under the direct supervision of Dr. Mark S. Dortch, Chief, WQCMB, and under the general supervision of Dr. Richard E. Price, Chief, EPED, and Dr. John Harrison, Director, EL. This report was reviewed by Drs. Holland and Cullinane.

At the time of publication of this report, Director of WES was Dr. Robert W. Whalin. Commander was COL Bruce K. Howard, EN.

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Conversion Factors, Non-SI to SI Units of Measurement

Non-SI units of measurement used in this report can be converted to SI units as follows:

Multiply	By	To Obtain
feet	0.3048	meters
miles (U.S. statute)	1.609347	kilometers
pounds (mass)	0.4535924	kilograms

1 Overview

The U.S. Army Engineer Waterways Experiment Station (WES) Groundwater Modeling Team initiated a project in fiscal year 1992 (FY92) to determine the state of groundwater modeling as applied to Army remediation needs.

The evaluation of groundwater models against observations from well-defined, multidimensional, field- or large-scale laboratory experiments will provide the user community with a tool to promote the acceptance of modeling efforts. Thorough evaluations will provide the older "mature" codes the confirmation and acceptance that until now has eluded them because they were applied with mixed success in groundwater problems.

The objective of this report is to provide detailed and complete technical guidance to the Department of Defense (DoD) environmental restoration community in the selection of appropriate groundwater models and their application to subsurface remediation issues. This is an expressed need of DoD personnel responsible for environmental restoration of military installations.[1] An assessment of the assets and limitations of selected codes for application to DoD groundwater remediation efforts is needed to assist decision makers in the selection of the best modeling approach in support of remedial design/operation.

Code selection and application to remediation efforts likely will require defense in any judicial proceedings. The use of thoroughly and successfully evaluated models establishes the technical and institutional validity of model selection in such potential litigations.

Results of this evaluation exercise will provide evidence that can be used by practitioners to advocate (or protest) the use of a particular model for a project. Use of an appropriate and well-documented model for remediation design will assist in negotiations with regulatory agencies, other responsible parties, or subcontractors.

Guidance regarding the minimal (and preferred) documentation needed for the application of any groundwater modeling project is essential. This guidance includes suggestions regarding the minimal amount and types of

[1] As expressed at the ARMY Groundwater Modeling Uses and Needs Workshop, 31 March -1 April, 1992, Denver, CO.

information that should be recorded (if not included) in official documents detailing the application of numerical modeling to a remediation project. Such information should include, for example, descriptions of and rationale for the perceived conceptual model, numerical model selection and implementation, selection of calibration targets or tolerances, quantitative calibration assessment, and sensitivity analyses.

Results from a rigorous, quantitative evaluation of a select suite of groundwater flow and transport codes can be used as a pattern for future model application. This suite of codes will be sufficiently diverse to meet present Army needs.

2 Literature Review and Model Selection

Initial Screening

The initial screening was a broad review of available groundwater models and an assessment of Army modeling needs. The goal of the initial model inventory was to assemble a list of reasonably available codes. Obtaining information on many of the codes in the initial list was impeded by lack of widespread documentation (e.g., gray literature or proprietary codes). Appendix A contains the initial list of groundwater codes compiled as part of the literature review of this investigation. However, the list will require maintenance to include new and upgraded models and more information on existing models as such becomes available. The list was originally compiled as a "living document," which will be updated as part of future model evaluation reports. Groundwater modeling will continue to evolve for the foreseeable future, probably at an accelerating pace and so will the list of models. Monitoring this model development and providing guidance are important services DoD can provide to Army groundwater modeling efforts.

Groundwater model selection depends upon the complexity of the remediation problem, the stage of site evaluation, time and financial constraints, and the capability of the model user. No single code or model package approaches the complete coverage of the flow and transport processes relevant in remediation modeling. Most remediation efforts do not, however, require modeling of all possible transport processes, which is fortunate since the data are rarely available for such a level of modeling.

The objective of the literature review of groundwater models was to compile a guide that could provide the following:

a. An extensive list of existing groundwater models grouped in selected categories, including a brief description and source/vendor/distributor.

b. Identification of Army groundwater remediation problems and modeling requirements.

c. Identification of the transport processes requiring consideration in order to address required remediation modeling.

Classifications of Models

Existing models were classified according to their key flow and transport processes or special applications (Table 1). This classification was adopted in order to help the user identify appropriate groundwater models for their application. Currently most of the groundwater modeling applications deal with saturated flow modeling (pump and treat) and in some occasions saturated flow and transport simulations (Hadala et al. 1993). The above statement applies to both the Army, DoD, and in general and the private sector (Hadala et al. 1993; Geraghty and Miller 1992).

Table 1
Model Classification

Saturated (Flow and/or Transport)
Unsaturated (Flow and/or Transport)
Coupled Unsaturated/Saturated (Flow and/or Transport)
Multiphase (Flow and/or Transport)
Geochemical Models

Conditions (flow, media, and contaminants) are usually established early in the site assessment or remedial investigation process so that an informed model selection is possible. Knowledge of media properties such as hydraulic conductivity, porosity, and specific storage in addition to the flow domain allows the user to select a specific class of groundwater model to solve a distinct problem. As more site knowledge is acquired through the development of a conceptual model, the user can then select a code not only from a particular class of model but with special formulations to address the individual program.

Site knowledge such as the existence of homogeneous, heterogeneous, layered, isotropic, or anisotropic domain (aquifer) allows the user to narrow the selection process to those models whose assumptions satisfy the conceptual model. For example, to simulate a fairly homogeneous saturated confined aquifer, the user must select a model from a decision tree. The first level of decision would be between analytic or numerical models for saturated flow; the next decision level could be the dimension of the modeling approach (one-, two-, or three-dimensional); the following decision may be between flow or flow and transport models; and conceivably another decision level could involve transport processes to be included in the flow and transport models.

Knowledge acquired during the development of the conceptual model should drive the model selection process and vice versa.

Appendix A meets the first objective of the literature review by providing an extensive list of available groundwater models. Appendix A follows the classification of Table 1 with the addition to subcategories like analytic solutions. Categories not covered in this report are flow and transport in fractured media, bioremediation, inverse modeling, stochastic modeling, and optimization.

Models for bioremediation, inverse problems, optimization, stochastic modeling, and other special categories were beyond the scope of the current review. Reviews of models in these categories will be undertaken as part of other Groundwater Modeling Team efforts.

Hadala et al. (1993) document a first cut at identifying Army needs, problems, and modeling needs in remediating contaminated groundwater sites. The current effort provides the user a companion to a model's user guide. The document describes several model applications that can help the user in applying the evaluated codes to specific sites. In addition, the report reviews and evaluates several groundwater models that cleanup specialists might apply in the near future, thus providing a reference source.

Appendix B of this report is a summary of processes requiring consideration if remediation modeling of organic contaminants is going to be successful. Most of the transport models evaluated herein contain a subset of the processes described in Appendix B. The processes incorporated in each specific model will be described and discussed in the model evaluation section. In addition to the processes described in Appendix B, contaminant degradation is an important process. Most contaminant transport models include either a first order, a zero order, or a combination of first and zero order degradation rates. First and zero order degradation rates are relatively easy to incorporate in either numerical or analytic groundwater models.

Groundwater Modeling

The use of groundwater models, in particular numerical groundwater models, has escalated in recent years due in part to regulatory pressures, innovative technologies, and the high cost of intensive sampling. This section is a primer or review of saturated and unsaturated groundwater flow and transport. The emphasis is to present the mathematical formulations on which most current groundwater models are based. It is intended as a primer and a reference source.

Saturated

Groundwater flow in saturated media is based on Darcy's law. Darcy found that the one-dimensional flow of water through a pipe filled with sand is proportional to the cross-sectional area of the pipe and the head loss along the pipe and inversely proportional to the flow length (Fetter 1993). The mathematical formulation can be expressed as

$$Q = -KA\frac{dh}{dl} \tag{1}$$

where

Q = volumetric discharge

K = proportionality constant known as hydraulic conductivity

A = cross-sectional area

dh/dl = gradient of hydraulic head

Darcy's law can be expressed in terms of the specific discharge or Darcy's flux, q, which is the volume of water flowing per unit time through a unit cross-sectional area. Darcy's flux, q, is also defined as Q/A.

$$q = -K\frac{dh}{dl} \tag{2}$$

The specific discharge or Darcy's flux, q, represents the flow per unit cross-sectional area of the column or medium that also includes the solid matrix. The average velocity (seepage velocity) only considers the portion of the area available to flow, that is εA; thus, the average velocity, V, of the flow through a column is

$$V = \frac{Q}{\varepsilon A} = \frac{q}{\varepsilon} \tag{3}$$

Darcy's law is applicable for most groundwater flow conditions but begins to deviate from observations at high-flow velocities (small Reynolds number) that may be encountered near large pumping and recharging wells, flow through cavernous material such as limestone, and flow through breakwaters constructed of gravel or large stones. Flow through very fine grained media (usually not in aquifers) is also not described well by Darcy's equation (Bear and Verruijt 1987).

The hydraulic conductivity or coefficient of proportionality, K, can be defined as the specific discharge per unit hydraulic gradient and has units of velocity (L/T). Hydraulic conductivity depends on both fluid properties and soil matrix properties. Fluid properties that influence the hydraulic conductivity are the density and viscosity of the fluid. The relevant solid matrix property is related to grain-size distribution, grain shape, surface area, and porosity. Thus the hydraulic conductivity can be expressed in terms of the permeability, which only depends on the soil properties

$$K = \frac{k\rho g}{\mu} = \frac{kg}{\nu} \tag{4}$$

where

g = acceleration of gravity

ρ = liquid density

μ = liquid viscosity

ν = kinematic viscosity

k = permeability of porous medium

Bear and Verruijt (1987) and Maidment (1993) provide typical values for hydraulic conductivity and permeability for different aquifer materials.

A porous medium is said to be homogeneous with respect to permeability if the permeability is the same at all points. Otherwise, the porous medium is said to be heterogeneous; permeability varies from point to point. If the permeability is independent of direction, then the porous medium is

said to be isotropic. If the permeability varies with direction, then the medium is said to be anisotropic. Both permeability and hydraulic conductivity (as well as other porous media properties) can exhibit anisotropy. Aquifers are often anisotropic.

Hydraulic gradient is a vector, having both magnitude (a value) and direction. Hydraulic conductivity is a tensor, thus described by nine components. If the coordinate system is oriented along the principal axes, the tensor becomes

$$K = \begin{matrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{matrix} \tag{5}$$

and for the isotropic case becomes $K = K_{xx} = K_{yy} = K_{zz}$. For isotropic porous medium, Darcy's law in three dimensions becomes

$$q = -K\frac{\partial h}{\partial x} - K\frac{\partial h}{\partial y} - K\frac{\partial h}{\partial z}$$

or (6)

$$q = K\nabla h$$

The movement of contaminants in saturated groundwater flow can be described according to Mercer and Waddell (Maidment 1993) as a combination of advection of the contaminant with the water flowing through an aquifer, dispersion of the contaminant, and sources and sinks of the contaminant through the aquifer. Mass balance equations that describe the above processes are the basis of most saturated groundwater flow and transport computer codes. Mercer and Waddell describe a typical mass balance as:

Dispersion + advection by natural flow + advection by pumping + other sources and sinks = rate of change of mass of contaminant stored in the aquifer

The advection-dispersion equation for contaminants in saturated groundwater flow can be written as:

$$\left[\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\right]$$

$$-\left[\frac{\partial}{\partial x}(v_x C) + \frac{\partial}{\partial y}(v_y C) + \frac{\partial}{\partial z}(v_z C)\right] \tag{7}$$

$$q_{in}C^* - q_{out}C + R = \frac{\partial C}{\partial t}$$

where

D_i = dispersion coefficient in direction i (x, y, z)

v_i = average velocity in direction i

q_{in} = volumetric flow rate of water source

q_{out} = volumetric flow rate of water sink

R = chemical source or sink

C = contaminant concentration

C^* = contaminant concentration of source

The dispersion coefficient, D_i, in Equation 7 is what Fetter (1993) calls the hydrodynamic dispersion coefficient and is a combination of molecular and mechanical dispersion. In the direction of the flow $D_i = D_L$, the hydrodynamic dispersion coefficient is parallel to the principal direction of flow (longitudinal). Equation 8 shows the relationship between hydrodynamic dispersion and dispersivity for porous media.

$$D_L = \alpha_L v_i + D^* \tag{8}$$

where

D^* = effective diffusion coefficient, which is related to molecular diffusion coefficient (Fetter 1993)

α_L = longitudinal dynamic dispersivity

v_i = average velocity in direction i

The Peclet number is a useful dimensionless number that can relate the effectiveness of mass transport due to advection to that due to dispersion. Peclet numbers indicate which process is dominant in groundwater mass transport. The Peclet number is defined as:

$$Pe = \frac{v_x L}{D_L} = \frac{v_x d}{D_m} \tag{9}$$

where

d and L = characteristic flow lengths

D_m and D_L = molecular and longitudinal dispersion coefficients, respectively

At Peclet numbers above 5, advection dominates; at Peclet numbers below 0.02, diffusion dominates (Fetter 1993). Peclet numbers also play an important role in the selection of a particular numerical method for solving groundwater transport problems.

The mass transport equation (7) for contaminants in groundwater includes a term called R, defined as the chemical source and/or sink. The sources and sinks or mechanisms of contaminant removal/addition to groundwater may be separated into two principal processes: sorption and

reactions. Sorption includes all the processes by which solutes cling to solid or porous medium surfaces. Sorption causes some contaminants to move much slower through an aquifer than the groundwater that is transporting them. This effect is called retardation. Remediation may, however, take longer in presence of sorption. Reactions, on the other hand, decrease or increase the contaminant concentration but may not necessarily slow the rate of contaminant movement.

Appendix B further examines sorption and reactions. Fetter (1993) provides an extensive discussion of reactions, reaction rates, and sorption, including some example cases. Maidment (1993), Lyman, Reehl, and Rosenblatt (1982), Montgomery and Welkom (1989), and Montgomery (1991) include estimates and parameter ranges for sorption and reactions of certain contaminants in groundwater.

Unsaturated

All models describing the movement and fate of chemicals in the unsaturated or vadose zone are based on the principles of mass conservation. The vadose zone extends from the soil surface to the water table, including the capillary fringe. In the capillary fringe, the pores may actually be saturated. The main discernable characteristic of the vadose zone is that the pore water pressures are usually negative. Vadose zone hydrology/ hydraulics are different from saturated zone hydrology/hydraulics because of the presence of air in the pore space.

Soil water movement controls the supply and distribution of water in the soil matrix. The ability of a soil to move or distribute water is a function of the soil properties. Hydraulic conductivity and water-retention characteristics are soil properties that affect the movement of water and transport of contaminants in soil systems. Hydraulic conductivity is a measure of the soil's ability to transmit water. The soil's ability to store and release water is measured by its water-retention characteristics.

Soil-water content or volumetric soil-water content can be expressed as:

$$\theta = \frac{V_w}{V_t} = \frac{W_w \rho_b}{W_d \rho} = \varepsilon S_w \tag{10}$$

where

$$\varepsilon = 1 - \frac{\rho_b}{\rho_p} \tag{11}$$

where

θ = volumetric water content, L^3/L^3

V_w = volume of water, L^3

V_t = total volume of soil, L^3

W_w = weight of water, M

ρ_b = bulk density of soil, M/L^3

W_d = weight of dry soil, M

ρ = water density, M/L^3

ε = total porosity (fraction)

S_w = water saturation (saturation), $0 \leq S_w \leq 1$

ρ_p = particle density, M/L^3

The soil-water retention curve is the relationship between the soil-water content and the soil matric potential. The water-retention characteristic is also known as the moisture characteristic, moisture retention, soil-water characteristic, or capillary pressure-saturation curve. Matric potential is synonymous with capillary potential, soil-water suction, capillary pressure head, tension, pressure potential, and matric pressure head, although the sign or the units of the terms may differ. Matric potential is the measure of the energy status of water in the soil and is a component of the total soil-water potential (Maidment 1993). Total soil-water potential, ϕ, is described as:

$$\phi = h_g + h_p + h_o + h_{ec} \tag{12}$$

where

h_g = gravitational potential

h_p = matric potential

h_o osmotic potential

h_{ec} = electrochemical potential

Since electrochemical potential and osmotic potential are relatively constant within the soil matrix, their gradient will zero; thus both can be ignored (Fetter 1993). After neglecting osmotic and electrochemical potential, the total soil moisture potential is reduced to the sum of the matric potential h_p or Ψ and gravitational potential h_g or z:

$$\phi = \Psi(0) + z \tag{13}$$

Matric potential can be expressed as capillary pressure with units of energy per unit volume, ϕ_{ev} (L/MT^2), as head with units of energy per unit weight or length, ϕ_{ew} (L), or as energy per unit mass, ϕ_{em} (L^2/T^2). Most common units for total potential and pressure potential include atmospheres and centimeters of water. Figure 1 shows matric potential and typical units, where the subscripts *ev* = energy per unit volume; *ew* = energy per unit weight; and *em* = energy per unit mass.

Equations	Units	TypicalUnits
$\phi_{ev} = p_c + \rho g z$	$(\frac{L}{MT^2})$	$\frac{newtons}{m^2}$ or $\frac{joules}{m^3}$
$\phi_{ew} = \frac{p_c}{\rho g} + z$	(L)	$cm of H_2O$
$\phi_{ew} = h + z$	(L)	$cm of H_2O$
$\phi_{em} = \frac{p_c}{\rho} + gz$	$(\frac{L^2}{T^2})$	$\frac{joules}{kg}$

Figure 1. Matric potential expressions and default units

The most common models or functions used to relate the water content to matric potential are those of Brooks and Corey, Campbell, and van Genuchten (Maidment 1993). Figure 2 describes the mathematical relationships for several moisture-retention models. Maidment (1993), Norfzinger et al. (1989), and Lappala, Healy, and Weeks (1987) contain typical values for the fitted parameters in the models described in Figure 2.

The hydraulic conductivity in unsaturated flow is a nonlinear function of volumetric soil-water content. At the same time, the soil-water content is a function of the matric potential. Unsaturated soils have a lower hydraulic conductivity because some of the pores are filled with air and do not transmit water. Water moves in the unsaturated zone only through wetted pores. Figure 3 describes the mathematical formulations for several hydraulic conductivity matric potential relationships (models) and hydraulic conductivity volumetric soil moisture models.

Most current unsaturated zone models incorporate a form of Darcy's law for flow through porous media. The Buckingham/Darcy law is one of the most common:

$$q = -K(\Psi)\nabla(\phi) \tag{14}$$

where

q = soil moisture flux

$K(\Psi)$ = unsaturated hydraulic conductivity at a given Ψ

$\nabla(\phi)$ = gradient of total soil-water potential, ϕ

Water-Retention Functions

1. Haverkamp et al. (1977)

$$\theta(h) = \theta_{res} + \frac{\alpha[\theta_s - \theta_{res}]}{[\alpha + (\ln|h|)^b]} \qquad \text{for } h < -1$$

$$\theta(h) = \theta_s \qquad \text{for } h \geq -1$$

2. van Genuchten (1980)

$$\theta(h) = \theta_{res} + \frac{[\theta_s - \theta_{res}]}{[1 + (\alpha|h|)^b]^m} \qquad \text{for } h < 0$$

$$\theta(h) = \theta_s \qquad \text{for } h \geq 0$$

where $m = 1 - 1/b$

3. Brooks and Corey (1964)

$$\theta(h) = \theta_{res} + [\theta_s - \theta_{res}]\left\{\frac{p_e}{h}\right\}^b \qquad \text{for } h < p_e$$

$$\theta(h) = \theta_s \qquad \text{for } h \geq 0$$

4. Campbell (1974)

$$\theta(h) = \theta_s \left(\frac{p_e}{h}\right)^{\frac{1}{b}} \qquad \text{for } h < p_e$$

$$\theta(h) = \theta_s \qquad \text{for } h > p_e$$

θ_s = saturated water content or porosity
θ_{res} = residual water content
$\theta(h)$ = volumetric water content at matric potential h
p_e = entry or bubbling capillary pressure
b = empirical parameter

Figure 2. Soil-water retention relationships

Hydraulic Conductivity Functions

1. Haverkamp et al. (1977)

$$K(h) = K_s \frac{\alpha}{\{\alpha + |h|^b\}} \qquad \text{for } h < 0$$

$$K(h) = K_s \qquad \text{for } h \geq 0$$

2. van Genuchten (1980)

$$K(h) = K_s \frac{\{1 - (\alpha|h|)^{b-1} \; [1 + (\alpha|h|)^b]^{-m}\}^2}{\{1 + (\alpha|h|)^b\}^{\frac{m}{2}}} \qquad \text{for } h < 0$$

$$K(h) = K_s \qquad \text{for } h \geq 0$$

where m = 1 - 1/b

3. Exponential

$$K(h) = K_s \exp(bh) \qquad \text{for } h < 0$$

$$K(h) = K_s \qquad \text{for } h \geq 0$$

4. Campbell (1974)

$$K(h) = K_s \left(\frac{P_e}{h}\right)^{2 + \frac{(\alpha + 2)}{b}} \qquad \text{for } h < p_e$$

$$K(h) = K_s \qquad \text{for } h \geq p_e$$

K(h) = soil hydraulic conductivity at matric potential h
K_s = saturated hydraulic conductivity
p_e = entry or bubbling capillary pressure
b = empirical parameter

Figure 3. Hydraulic conductivity relationships

The governing differential equation for fluid flow through porous media is obtained from continuity and Darcy's law. A general form of the mass balance can be expressed as:

$$\left\{S_w\left[\rho(1-\varepsilon)\alpha + \varepsilon\rho\beta\right] + \varepsilon\rho\frac{\partial S_w}{\partial \phi_{ev}}\right\}\frac{\partial \phi_{ev}}{\partial t} + \varepsilon S_w\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} - \nabla\bullet K\nabla\phi_{ev} - Q = 0 \quad (15)$$

where

ϕ_{ev} = total pressure head, $p_c + \rho gz$

K = hydraulic conductivity tensor

Q = flow point sources/sinks

α = pore volume compressibility

β = liquid compressibility

C = solute concentration

The term $dS_w/d\phi_{ev}$ is the specific moisture capacity and relates to the soil's pressure saturation relationship in the unsaturated zone. Unsaturated codes solve Equation 15 with appropriate boundary and initial conditions for the pressure (matric head) distribution. The velocity field is then estimated from the pressure head and Darcy's law (Darcy-Buckingham). The velocity field is used to solve for the associated contaminant transport. A general form of the contaminant mass balance in unsaturated porous media can be written as:

$$\frac{\partial}{\partial t}(\varepsilon\rho S_w C) + \frac{\partial}{\partial t}(\rho_b S) + \nabla\bullet(\varepsilon\rho S_w qC) = \nabla\bullet(\varepsilon\rho S_w D)\bullet\nabla C + \varepsilon\rho S_w\Psi + \rho_b\Psi_s\ Q_pC^* \quad (16)$$

where

C = solute concentration in liquid phase

S = solute concentration on solid phase

ρ_b = soil bulk density

D = tensor, which includes both diffusion and dispersion

Ψ = rate of solute degradation/production in liquid phase

Ψ_s = rate of solute degradation/production in solid phase

Q_p = rate of liquid injection/withdrawal

C^* = solute concentration in fluid source/sink

Equilibrium sorption models can be used to define the solid phase concentration in terms of the liquid phase concentration, C. Three equilibrium

sorption isotherms are described in Appendix B, Part 1; in all three models, the solid phase solute concentration, S, is a function of $C(S = f(C))$. The general equation for sorption is:

$$\frac{\partial S}{\partial t} = f(C)\frac{\partial C}{\partial t} \tag{17}$$

where $f(C)$ is the solute concentration in the solid phase and is a function of fluid concentration, C.

The production/degradation terms for both liquid and solid phases account for chemical, biological, and/or physical reactions in the soil water or soil surface. The production/degradation rate for the solute in liquid phase is usually assumed as either first order or zero order:

$$\Psi = \lambda_1 C$$

or (18)

$$\Psi_s = \lambda_0$$

where λ_1 is the first-order rate constant, and λ_0 is the zero-order rate constant for the liquid phase. The solute rate in the solid phase rate is analogous:

$$\Psi_s = \gamma_1 S \tag{19}$$

where γ_1 is the first-order rate constant for the solid phase. Equation 19 can be written in terms of the solute in the liquid phase assuming linear sorption:

$$\Psi_s = \gamma_1 K_d C \tag{20}$$

where K_d is the linear partition coefficient, discussed in Appendix B, and all other terms have been previously defined. Degradation refers to reactions that decrease the solute; production refers to increase due to formation of the solute.

Model Selection

The initial list of models considered for evaluation is included in Appendix A. The list was reduced to a manageable suite, and the shorter list of models were further evaluated and summarized in this document. Criteria for this model screening were defined based primarily on current and anticipated Army needs (Hadala et al. 1993). The criteria used to select the models for the short list were the following:

a. Model and code are well documented.

b. Model has been previously tested.

c. Code/model meets the Army groundwater cleanup needs.

d. Source code is available.

e. Code is in the public domain.

The first criterion allowed selection of codes that are mature. Mature codes have fewer errors, have larger database of users, and have been applied to a variety of problems. The documentation of mature codes is usually satisfactory; if the code has undergone significant revisions, the documentation tends to be good. Some of the codes that were selected are not mature codes, but other factors influenced their selection.

The selection of the codes for further evaluation was influenced by previous model evaluations (Celia, Gray, and Hassanizadeh 1992; van der Heijde and Elnawawy 1992; Beljin 1988; Kincaid and Morrey 1984; Morrey, Kincaid, and Hostetler 1986; Wagner and Ruiz-Calzada 1987) and groundwater model reviews (Moskowitz et al. 1992; OSWER 1989, 1990; Mangold and Tsang 1991; Faust and Mercer 1980; Mercer and Cohen 1990; and Geraghty and Miller 1992). Beljin (1988) evaluated three codes, SEFTRAN, MOC, and RANDOM WALK, two of which were selected for further evaluation in this effort. The selection of codes that were previously evaluated and are very popular allows the authors to confirm the previous evaluation/validation and provides additional knowledge to future users.

Hadala et al. (1993) and Geraghty and Miller (1992) found that MODFLOW was the most used code in both Army and the U.S. Environmental Protection Agency (EPA) groundwater communities, respectively. Other popular codes from the surveys were RANDOM WALK and USGS-MOC. PRZM II was selected because it is the only unsaturated zone model that includes contaminant interaction in the root zone. Three coupled unsaturated-saturated zone models, FEMWATER/LEWASTE, VS2DT, and SUTRA, were selected because of their ability to solve both unsaturated and saturated zone problems. An additional reason for selecting FEMWATER/LEWASTE was its selection as the code of choice for wellhead protection analysis by EPA. MOFAT was selected because it is one of the few compositional multiphase flow models for which source code is available in the public domain.

The codes selected for further evaluation were grouped according to the classification of Table 1. The list of models evaluated is presented in Table 2. The codes were recommended for evaluation because of their popularity, maturity, properties, and/or flow and transport processes and pathways. CSU-GWFLOW and TRANSPORT evaluation will be documented in a contractor report.

Table 2
Models Selected for Further Evaluation

Saturated (Flow and/or Transport)	Unsaturated (Flow and/or Transport)	Coupled Unsaturated/ Saturated (Flow and/or Transport)	Multiphase
MOC	UNSAT1	FEMWATER	MOFAT (MOTRANS)
MODFLOW	CHEMFLOW	LEWASTE	
MT3D	PRZM II	SUTRA	
PLASM		VS2DT	
RANDOM WALK/RAND3D			
CSU-GWFLOW			
CSU-TRANSPORT			

Model Evaluation, Verification, and Validation

The purpose of the model evaluation is to provide an independent assessment on the applicabilities and limitations of the selected codes in solving groundwater contamination problems. The evaluation described in this report is a first step in a series of stages that constitute a validation protocol. In the first step, computer code, mathematical formulations, and numerical formulations were tested and evaluated. The testing included examples included with the code, problems described in the literature, and experimental data. All models were not subjected to the three levels of testing due to lack of either experimental data or available analytical solutions. Lack of available analytic solutions applies to both unsaturated flow and transport and multiphase flow.

The evaluation effort includes scrutiny of the code structure and performance evaluation relative to appropriate problems for which analytical solutions are available. The models were evaluated independently, and their performance in matching both flow and transport, as applicable, is documented. The summary on each evaluation includes the following:

a. Model description.

b. Platform for evaluation (personal computer (PC), workstation, mainframe).

c. Model performance in solving example problems included with the code.

d. Modifications, if any, for the evaluation.

e. Model performance in solving the "typical" scenarios: inputs, results, and comparisons.

f. Recommendations.

Similar evaluations/verifications have been proposed by State and Federal agencies. The State of Illinois has eight standards that must be met to accept a computer code for landfill permitting. The standards include the following: check model documentation; check mathematical equations; check numerical solution; model calibration against site-specific data; sensitivity analysis; mass balance checks; site-specific parameters shall be based on laboratory or field data; and nonsite-specific parameters need to be documented. Federal agencies like the EPA have hinted that future issuance of permits will be based on model application and testing, thus, the need of establishing testing and verification protocols.

Model verification is the assurance that the computer code correctly performs the operations specified in the numerical model (Beljin 1988). The key in model verification is to check the accuracy of the computational algorithm used in the numerical code to solve the mathematical formulations. A second objective is to make sure that the computer code is fully operational; that is, all options are operational.

Model validation provides the assurance that the algorithms embodied in the computer code correctly represent the physical processes or system to which the model is applied (Beljin 1988). Validation is an assessment of how the governing equations describe actual system behavior. A model is said to be validated when sufficient testing shows an acceptable degree of matching the actual systems.

Although several authors have shown some disagreement on the use of the terms validation and verification of groundwater models (Konikow and Bredehoeft 1978; Anderseon and Woessner 1992), the key is that the users and regulators need some level of confidence associated with a given model. The level of confidence can be called validation, verification, or just plain confidence level, but model confidence is a fundamental issue if meaningful modeling studies are to be performed. To achieve model confidence, a multistep or multitiered model testing protocol is proposed.

A multitiered assessment protocol consists of progressively evaluating the subject codes at rigorous levels of analysis. These levels are as follows:

a. Evaluation of code structure and process formulations.

b. Code performance on a set of problems for which analytical solutions are available.

c. Code performance on synthetic benchmarks (hypothetical scenarios).

d. Performance relative to laboratory experimental data (bench or artificial aquifer scale)

e. Code performance relative to well-controlled, field-scale experimental data.

Appropriate problems with analytical solutions are available for most model categories (Huyakorn and Pinder 1983). Highly reliable experimental data at the bench and field scale are limited or unavailable for several

categories of codes. All codes will be evaluated to assess their "ease-of-use" or lack thereof, memory requirements, hardware requirements, and other features.

3 Test Cases

Overview

The evaluation of groundwater codes requires the adherence to an established protocol as that proposed in the introduction of this report. In order to follow the proposed evaluation protocol, several test cases were selected. Each test case was selected to address a specific area of groundwater flow and transport modeling.

Three issues that influenced the choice of the test cases were as follows: cases have been previously used by other authors on previous model testing; the test cases are well known in the groundwater literature; and availability of an analytic solution—if no analytic solution is available, then a laboratory experiment was selected as a test case. Test cases were selected for saturated flow and transport, unsaturated flow, and coupled unsaturated and saturated flow.

The models were evaluated to different levels of code evaluation as described in Chapter 2. Saturated groundwater flow and transport models were evaluated to level two of the proposed testing protocol: code performance on a set of problems for which analytical solutions are available. Unsaturated and coupled unsaturated/saturated flow models were evaluated at levels one and four: code performance relative to laboratory experimental data. One saturated flow model, PLASM, was evaluated at levels one and three: code performance on synthetic benchmarks or hypothetical scenarios.

As a final note, all codes were evaluated to assess their "ease-of-use" in setting up or solving the test cases. Any model modification to solve the selected test cases will be documented in the model evaluation and/or discussion.

Saturated

The test cases selected for saturated groundwater flow and transport were three problems for which analytical solutions exist. The first criterion was in selecting the test problems previously used by other investigators: Beljin (1988) used them in evaluating four groundwater models, thus a

larger database of models can be compared using these three problems. The second selection criterion was that other researchers have also used the test cases in evaluating their codes (Pinder 1973; Wilson and Miller 1978; and Wagner, Watts, and Kent 1984). The third criterion is that the test cases meet the objective of checking the accuracy of computer models since an analytic solution exists for the three problems. The three test cases are as follows:

a. A continuous source in a constant flow field (Case 1).

b. A slug source in a constant flow field (Case 2).

c. A continuous source in a constant radial flow field (Case 3).

The three test cases correspond to example problems used in Beljin (1988). The cross reference to Beljin's report is as follows:

BM-I.3 (Case 1 in this report).
BM-I.4 (Case 2 in this report).
BM-I.5 (Case 3 in this report).

Case 1. Two-dimensional solute transport from a continuous point source in a uniform groundwater field. The test problem has been documented by other researchers (Pinder 1973; Wilson and Miller 1978; Wagner, Watts, and Kent 1984; Beljin 1988) and consists of the continuous injection of a contaminant from a point source or a well into an aquifer. As a result of the continuous injection, a plume develops downstream from the injection point and spreads out laterally. For a thin aquifer, vertical mixing should occur, and the concentration becomes uniform with depth in the aquifer. When uniform vertical occurs, the plume can be regarded as essentially two-dimensional.

The case history for the stated problem is based on the groundwater contamination with hexavalent chromium in South Farmingdale, Nassau County, New York (Wagner, Watts, and Kent 1984). The aquifer has a saturated thickness of 33.5 m with a porosity of 0.35. The average seepage velocity is 0.460 m/day and the estimated dispersivity values of α_L = 21.3 m and α_T = 4.27 m. The source of contamination consisted of three metal plating waste-disposal ponds by the Liberty Aircraft plant in South Farmingdale. The estimated mass rate of contaminants entering the aquifer has been estimated at 23.59 kg/day (Beljin 1988). Adsorption and degradation can be neglected since chromium is relatively conservative. A summary of the parameters is presented in Table 3.

Beljin (1988) used two grids in his evaluation, a coarse grid (Δx = 180 m, Δy = 60 m) and a fine grid (Δx = 60 m, Δy = 30 m). The Peclet number was 4.56 for the coarse grid and 2.91 for the fine one. For a time step of 100 days, the Courant numbers were 0.25 and 0.76 for the coarse and fine grid, respectively (Beljin 1988). Figure 4 shows a typical grid for Case 1 problem.

Case 2. Transport of a solute slug in a uniform groundwater flow field. The problem analyzes the two-dimensional solute transport due to a slug injection of a conservative contaminant into a uniform flow field. This

Table 3
Values of Physico-Chemical Parameters for Case 1

Aquifer saturated thickness, b	33.5 m	110 ft
Darcy Velocity, u	0.161 m/day	0.525 ft/day
Seepage velocity, $\bar{u}$	0.460 m/day	1.5 ft/day
Porosity, n	0.35	
Longitudinal dispersivity, α_L	21.3 m	69.9 ft
Transverse dispersivity, α_T	4.27 m	14.0 ft
Point source strength	23.59 kg/day	52 lb/day
QC_o per unit depth	704.0 g/day-m	
Retardation factor, R	1.0	
Decay constant, λ	0.0 1/day	

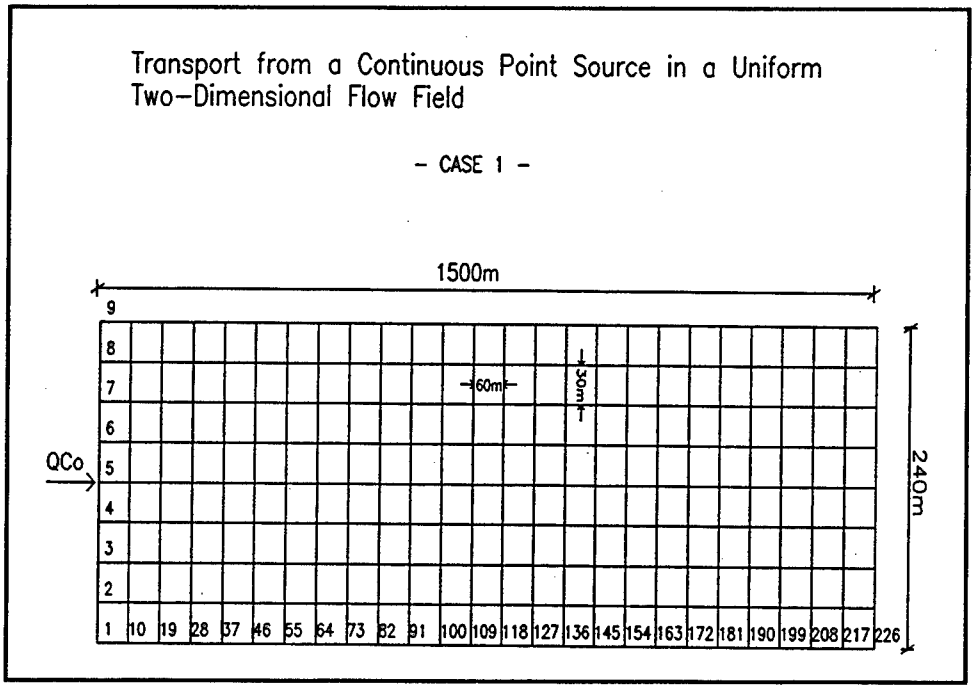

Figure 4. Two-dimensional transport from a continuous point source—Case 1

case is similar to Case 1 except for the boundary condition at the source. In Case 2, the mass per unit aquifer thickness is introduced at the boundary instantaneously.

The objective of this problem is to check the ability of groundwater codes to compute the position, size, and concentration distribution of the contaminant slug at a given time (Beljin 1988). The grid used by Beljin

(1988) consisted of rectangular elements with nodal spacing $\Delta x = \Delta y = 5$ m. The output from the groundwater models at Days 3.96, 10.59, and 16.59 is then compared against the analytical solution at the same times. A summary of the parameters for Case 2 simulation is presented in Table 4.

Table 4
Values of Physico-Chemical Parameters for Case 2

Darcy Velocity, u	2.0 m/day	6.56 ft/day
Seepage velocity, $\bar{u}$	5.71 m/day	18.75 ft/day
Porosity, n	0.35	
Longitudinal dispersivity, α_L	4.0 m	13.12 ft
Transverse dispersivity, α_T	1.0 m	3.28 ft
Solute mass per unit aquifer thickness, M	3.5 kg/m	2.35 lb/ft
Time, t	3,96, 10.59, 16.59 days	
Retardation factor, R	1.0	
Decay constant, λ	0.0 1/day	

Case 3. Solute transport from a continuous point source in a plane radial flow field. This problem considers the movement of a contaminant injected from a fully penetrating well. The injection is continuous, thus a continuous point source; however, the regional groundwater flow is negligible compared with the velocity created by the injection well. This problem is a near-well phenomena evaluation.

The objective of this problem is to test the ability of the groundwater code to correctly estimate the velocity field around an injection well. The model should be able to simulate the contaminant transport in nonuniform radial flow. This problem could be difficult for codes with only Cartesian coordinates.

The node spacing in Beljin's (1988) evaluation was uniform in the x- and y-directions, $\Delta x = \Delta y = 1$ m, and time step was 1 day. The summary for Case 3 parameters are presented in Table 5.

Unsaturated

Analytic solutions for unsaturated flow and transport were not available at the time of this evaluation; therefore, experimental test cases were used to measure the performance of unsaturated codes. Prill, Johnson, and Morris (1965) conducted several laboratory experiments investigating the

Table 5
Values of Physico-Chemical Parameters for Case 3

Well recharge rate, Q	25.0 m/day	4.59 gpm
Thickness of aquifer, b	10.0 m	32.80 ft
Porosity, n	0.25	
Lateral dispersivity, α_T	0.0 m	
Longitudinal dispersivity, α_L		
Test 1	0.300 m	0.984 ft
Test 2	0.150 m	0.492 ft
Test 3	0.015 m	0.049
Time, t		
Test 1	20.0 day	
Test 2	40.0 day	

effect of time on soil column drainage. In this evaluation, the data they acquired studying the drainage of a Fresno medium sand were used to evaluate unsaturated code performance. The data were previously used in validating unsaturated flow codes by Whisler and Watson (1968).

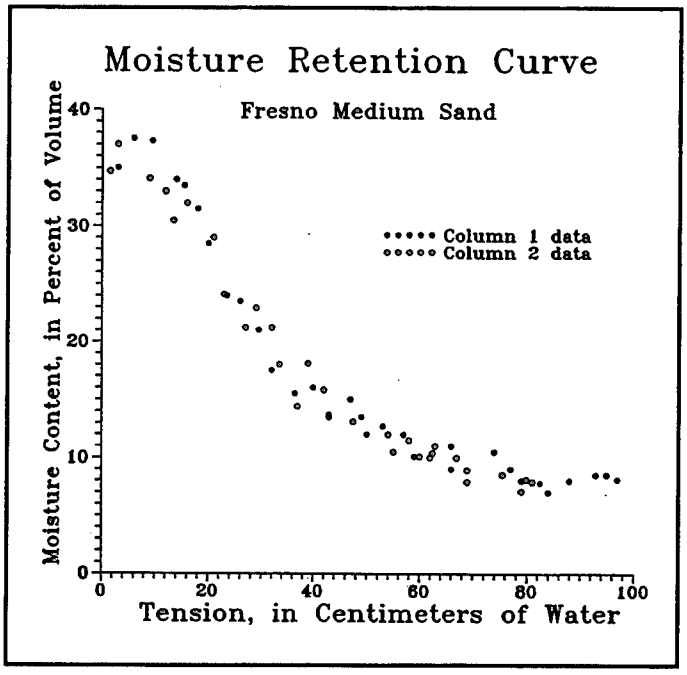

Figure 5. Experimental soil-water retention curve for Columns 1 and 2 (Prill, Johnson, and Morris (1965))

The study by Prill, Johnson, and Morris (1965) consisted of the drainage of a 140-cm soil column that was previously saturated with water. The soil column was packed with Fresno medium sand. The properties for the sand were evaluated, and the soil-water retention curve is shown in Figure 5. Moisture distribution and discharge data were collected in relation to time of drainage. The gravity drainage was conducted at constant temperature and lasted 4 days.

The simulation scenario consists of a soil column of packed Fresno medium sand draining from an initial moisture-content equivalent to saturation. The top of the column was at atmospheric pressure, and the bottom is open allowing for

free drainage. Figure 6 displays a typical column two-dimensional grid for drainage evaluation.

Figures 7, 8, and 9 show three moisture-retention models used in matching the Fresno medium sand experimental data by Prill, Johnson, and Morris (1965). The fitted parameters were then used in evaluating moisture movement with unsaturated codes. For the Fresno medium sand soil, the van Genuchten and Haverkamp moisture-retention models predict the pressure-moisture relationship better than the Brooks and Corey model. Other pressure-moisture power function relationships and typical fitted parameters can be found in Maidment (1993), Nofziger et al. (1989), and Lappala, Healy, and Weeks (1987). In addition, the International Ground Water Modeling Center (IGWMC) has several programs to estimate fitted parameters from experimental data.

One program used in this evaluation was SOIL, a nonlinear least squares analysis program to estimate soil hydraulic properties. It solves four moisture-retention models and fits the hydraulic conductivity to a straight line on a log-log curve. The software is interactive. Two other IGWMC programs for unsaturated soil property estimation are SOHYP and FP. All three models are part of the IGWMC collection.

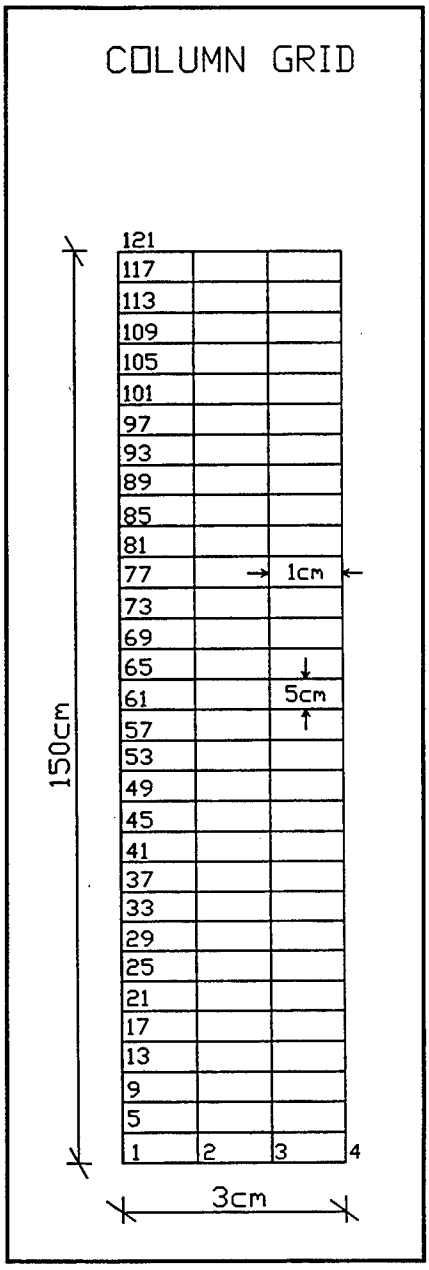

Figure 6. Two-dimensional column grid

Coupled Unsaturated/Saturated

The second test case used in evaluating unsaturated codes was a water table experiment by Vauclin, Khanji, and Vachaud (1979). The experimental apparatus consisted of a "sandbox" 3 m in length, 2 m in height, and 5 cm thick. The apparatus was used to study the two-dimensional, unsaturated, groundwater flow and recharge of a shallow water table aquifer.

A constant water level was maintained at a depth of 135 cm as shown on Figure 10. The left side and the bottom of the flow domain were no-flow boundaries (Neumann or Type 1 boundary) and the right boundary below 135 cm was set to constant head (Dirichlet or Type 2 boundary). The right side between 0 and 135 cm was a no-flow boundary as was the top from 50 cm to 300. A constant flux (Type 1 boundary or Neumann) of 14.8 cm/hr was applied at the soil surface over a width of 50 cm (0-50); the remaining soil surface was covered to prevent evaporation. Figure 11 shows a two-dimensional grid for Vauclin's experiment. The grid spacing corresponds to the experimental data.

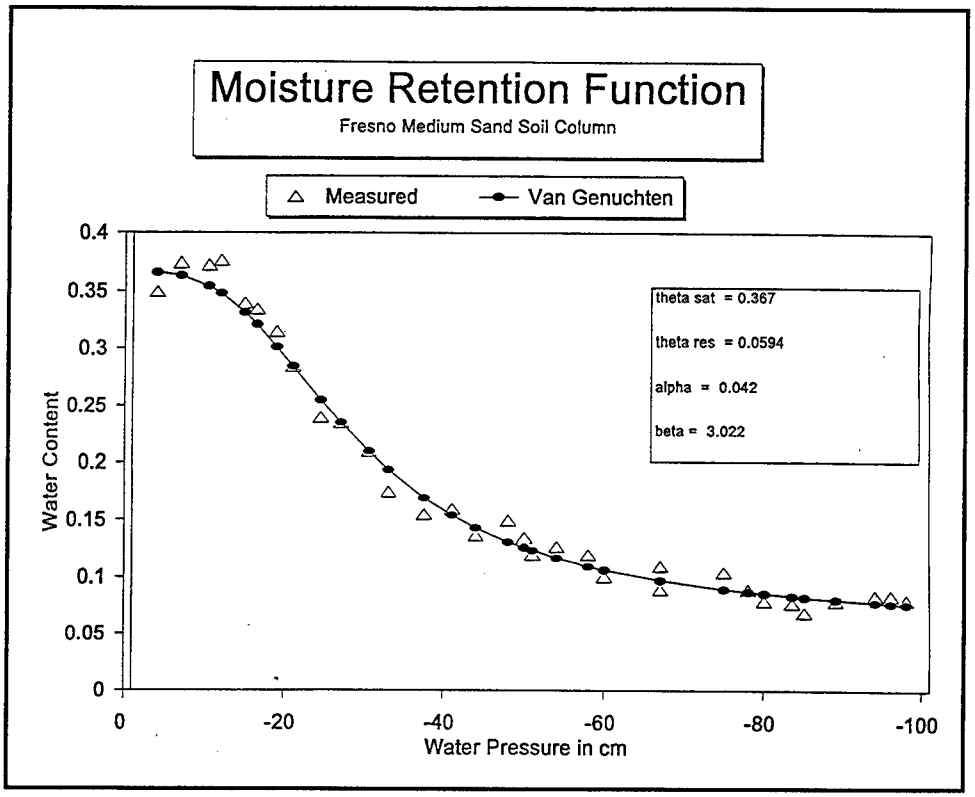

Figure 7. Moisture-retention function, van Genuchten model

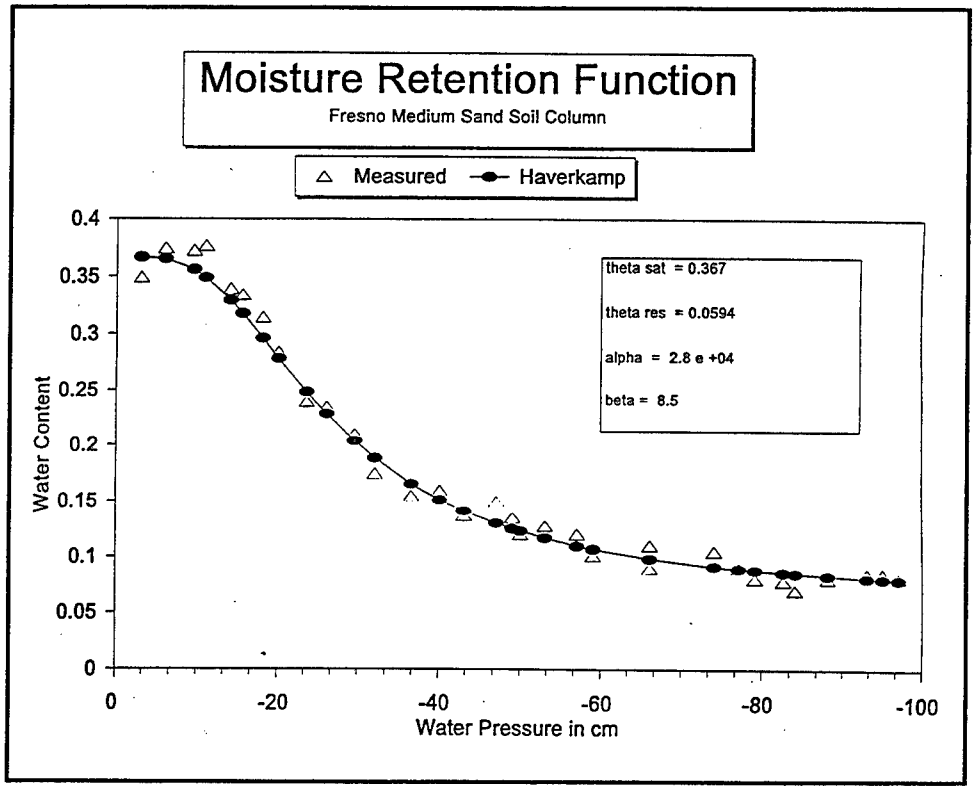

Figure 8. Moisture-retention function, Haverkamp model

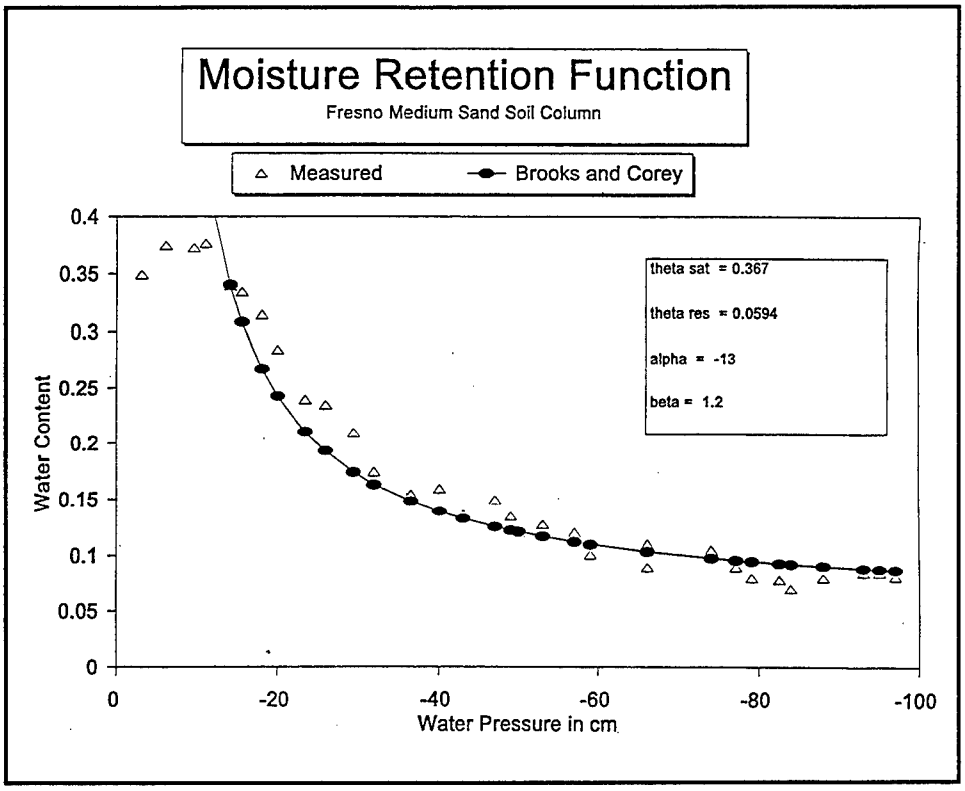

Figure 9. Moisture-retention function, Brooks and Corey model

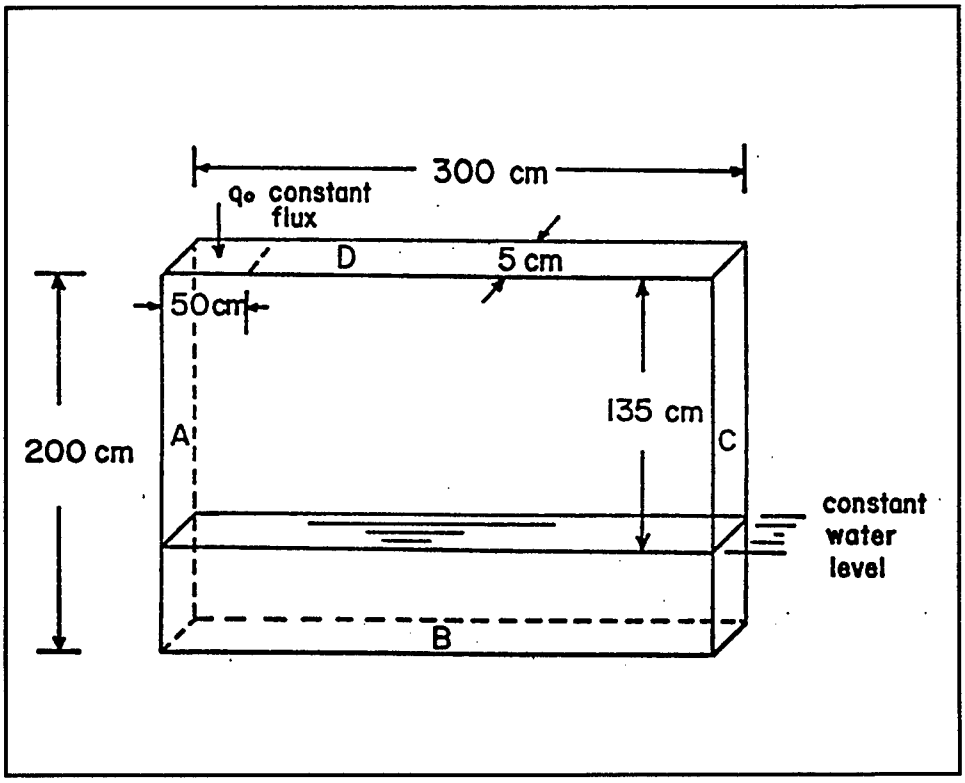

Figure 10. Schematic representation of Vauclin's infiltration experiment

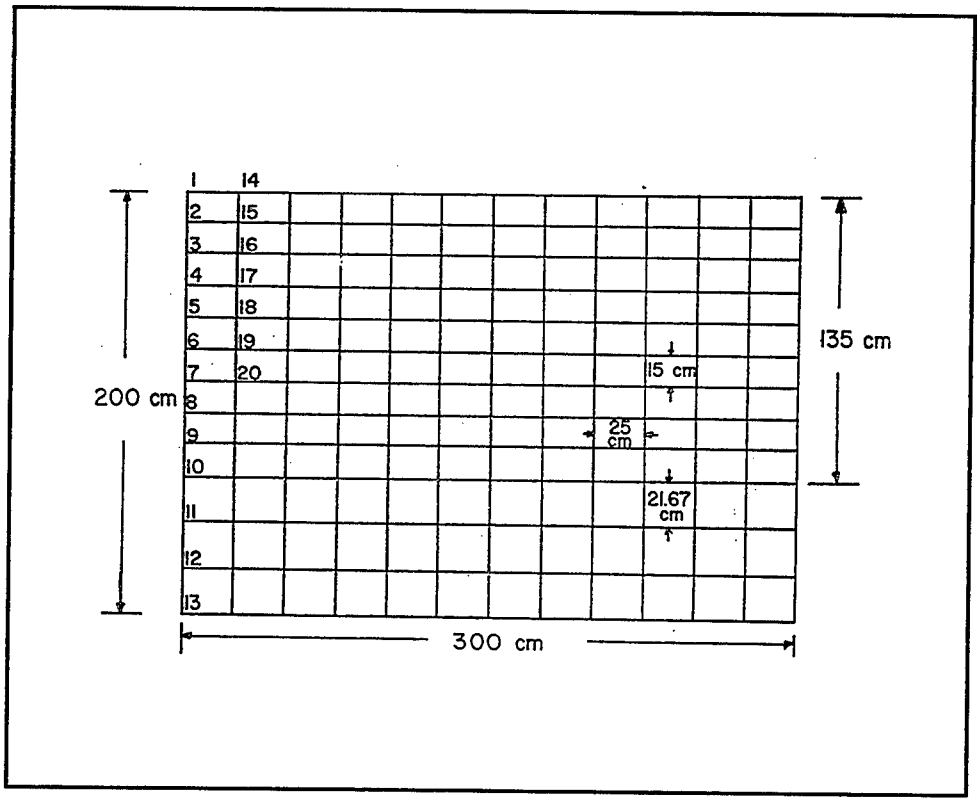

Figure 11. Two-dimensional grid for Vauclin's infiltration experiment simulations

The initial water distribution and pressure were measured experimentally prior to starting the recharge (Khangi 1975). Figure 12 shows the initial pressure distribution in the unsaturated and saturated zones. Data collected during the infiltration experiment included (a) volumetric water content, (b) water pressure over the entire flow domain, and (c) the position of the free water table at both left and right boundaries.

The results published by Vauclin, Khanji, and Vachaud (1979) and Khangi (1975) represent a detailed description of the porous media used in the infiltration experiment. The results represent one of the most comprehensive and detailed set of published data for unsaturated flow and media characterization. The water retention and hydraulic-conductivity relationships are shown in Figure 13. Figures 14, 15, 16, and 17 show three moisture-retention models and one hydraulic-conductivity model used in matching the fine-sand properties used in Vauclin's experiment. The fitted parameters were then used in evaluating moisture movement with unsaturated codes. For Vauclin's fine sand, similar to the Fresno medium sand, the van Genuchten and Haverkamp moisture-retention models predict the pressure-moisture relationship better than the Brooks and Corey model. Two hydraulic-conductivity relationships, Haverkamp and Campbell (Campbell 1974; Maidment 1993), were used to fit the parameters for Vauclin's sand. Figure 16 shows Haverkamp's hydraulic-conductivity match.

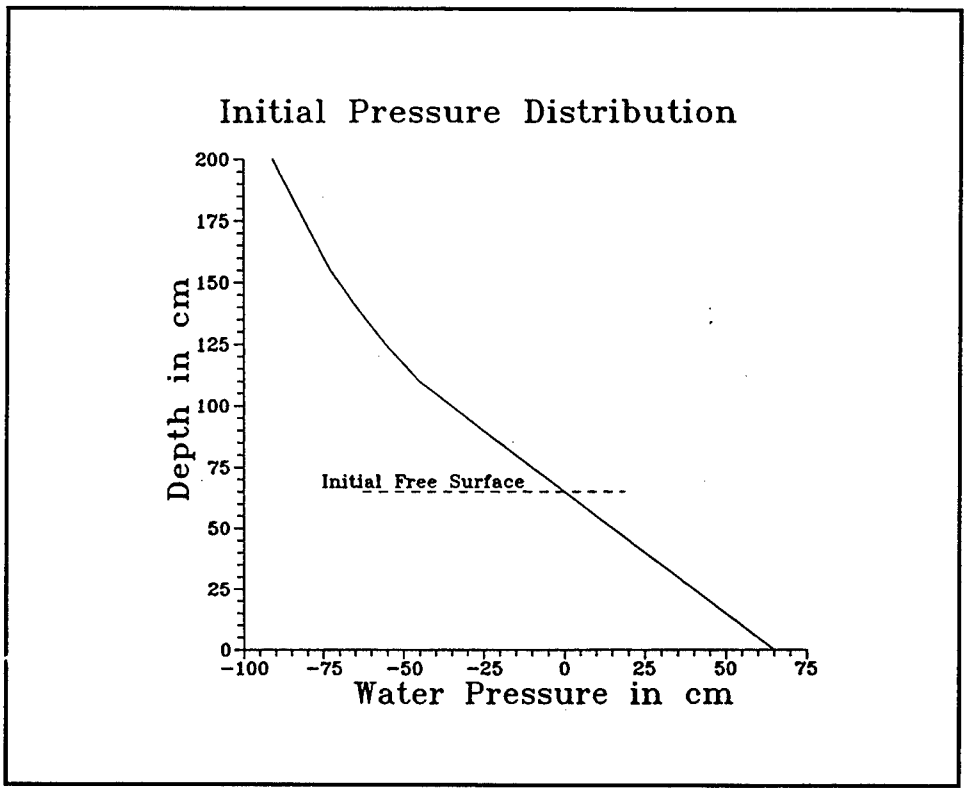

Figure 12. Initial pressure distribution

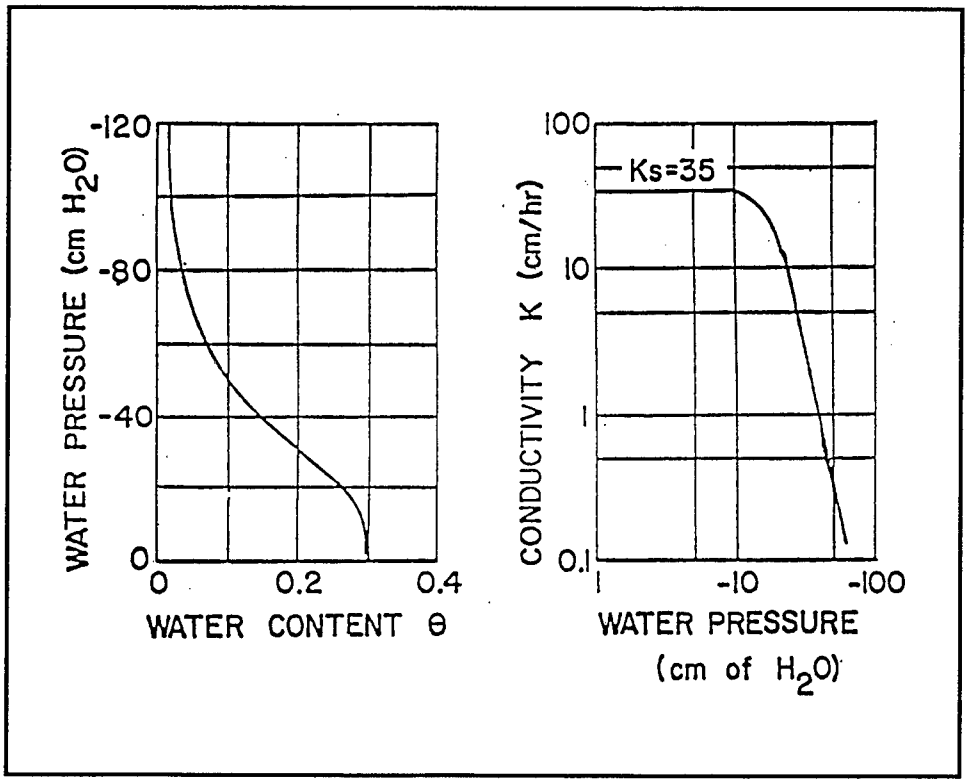

Figure 13. Experimental pressure and hydraulic-conductivity relationships (Vauclin, Khanji, and Vachaud 1979)

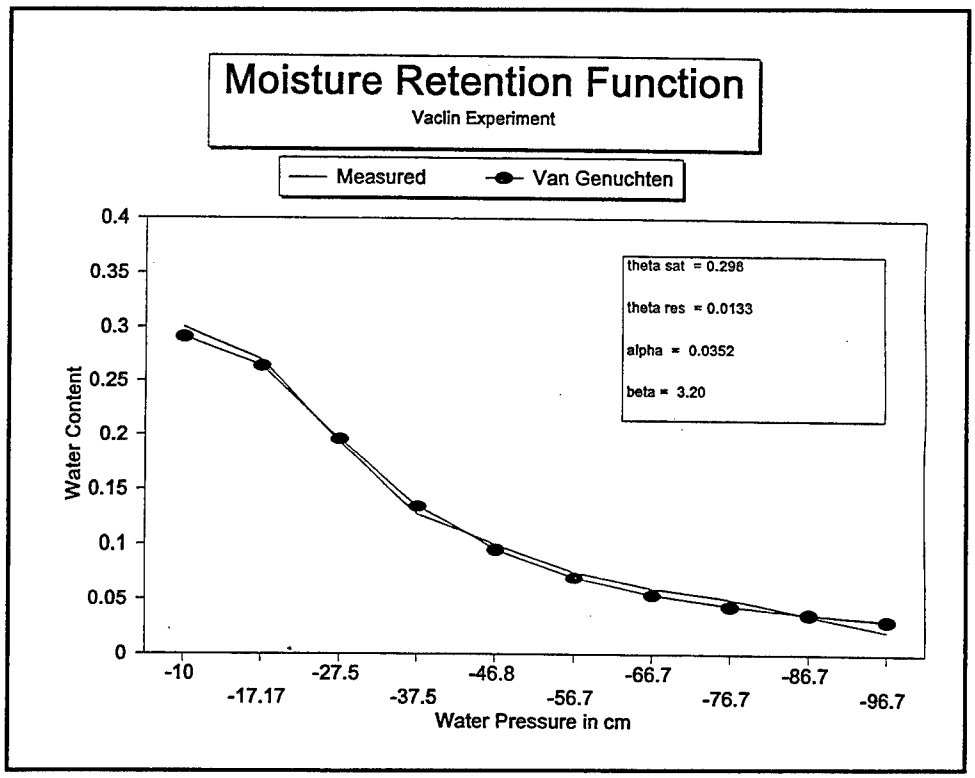

Figure 14. Moisture-retention function, van Genuchten model-Vauclin's experiment

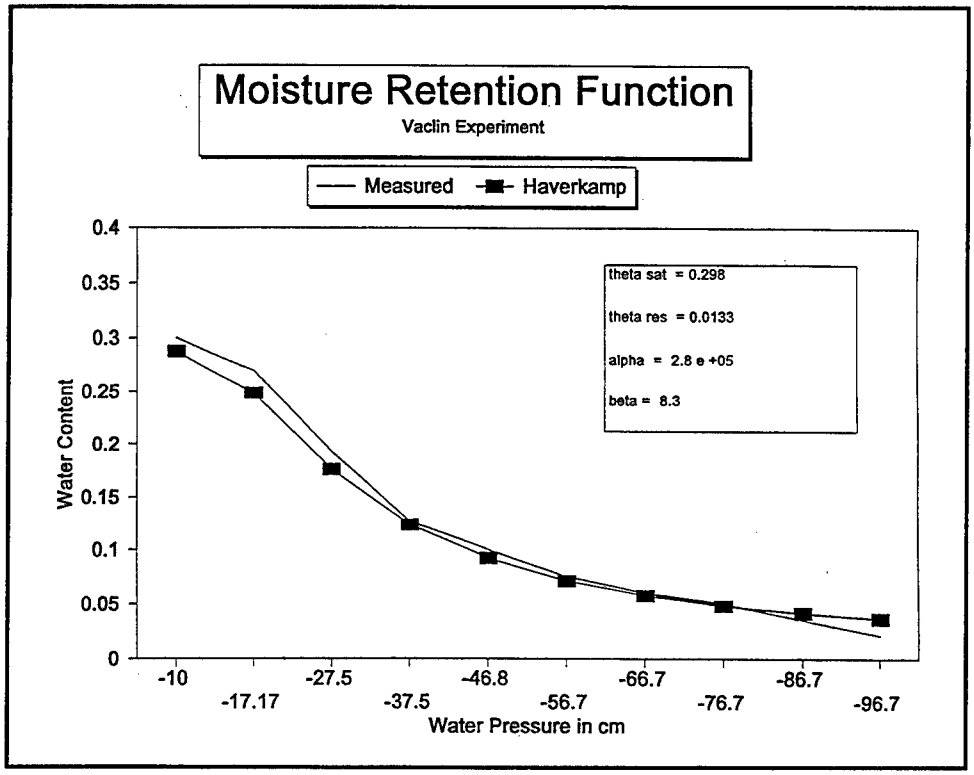

Figure 15. Moisture-retention function, Haverkamp model-Vauclin's experiment

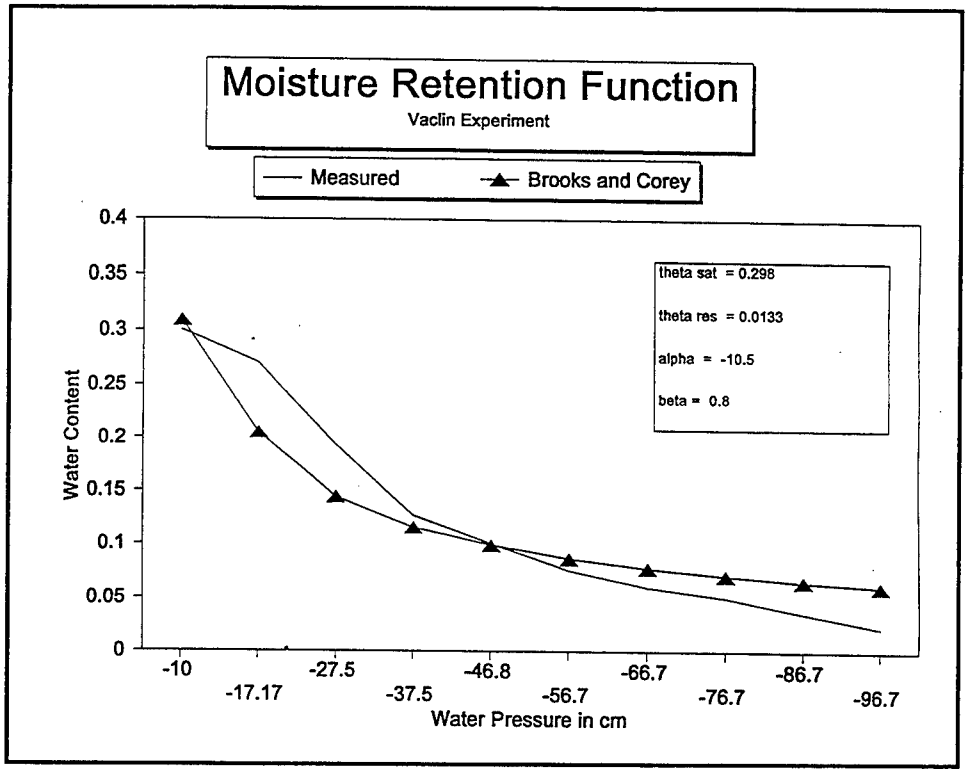

Figure 16. Moisture-retention function, Brooks and Corey model-Vauclin's experiment

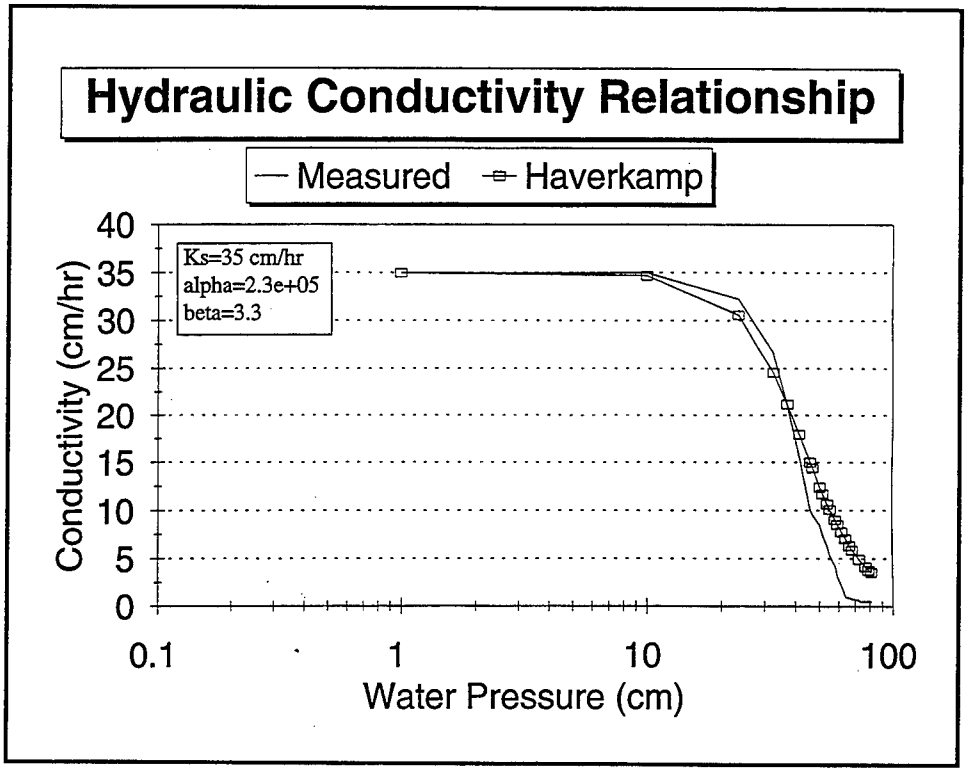

Figure 17. Hydraulic conductivity-pressure relationship, Haverkamp model-Vauclin's experiment

Hypothetical Scenarios

One hypothetical scenario was developed as an independent problem to serve as the base case scenario for testing the selected groundwater models. The test case was developed as a fairly simple case that could be solved by both analytic solution models as well as numerical models.

Figure 18 shows the plan view of the WES Example Problem 1. The example consists of a rectangular-shaped alluvial aquifer approximately 500 m long and 2,500 m wide. Figure 19 illustrates an aerial view of the test case. Boundary conditions are shown in Figure 19, and aquifer properties are presented in Table 6.

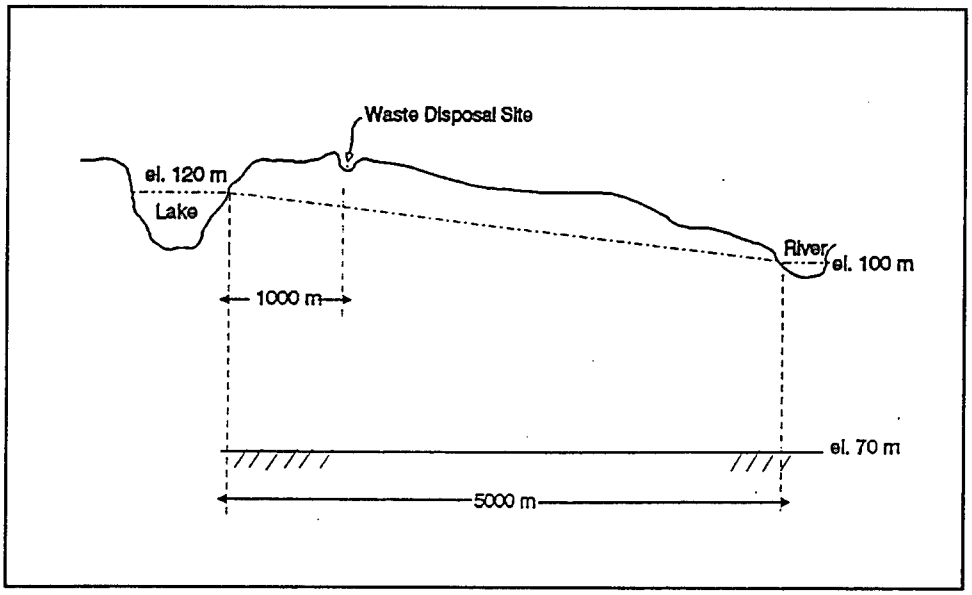

Figure 18. Schematic plan view of WES Example Problem 1

The aquifer is located between a river and a lake that provide constant head boundaries at the north and south ends of the aquifer (Figure 19). The lake level (head) is 120 m, and the river level (head) is 100 m. No-flow boundaries are created at the east and west sides of the aquifer due to an impervious rock outcrop. The contaminant source is a waste disposal pond located 100 m south of the lake.

The waste pond behaves like a constant point source to the aquifer. Leakage from the pond is 0.01 m^3/s, and the source concentration is 100 mg/ℓ. For the three-dimensional case, the waste pond is located 1,250 m from either no-flow boundary of the aquifer (Figure 19).

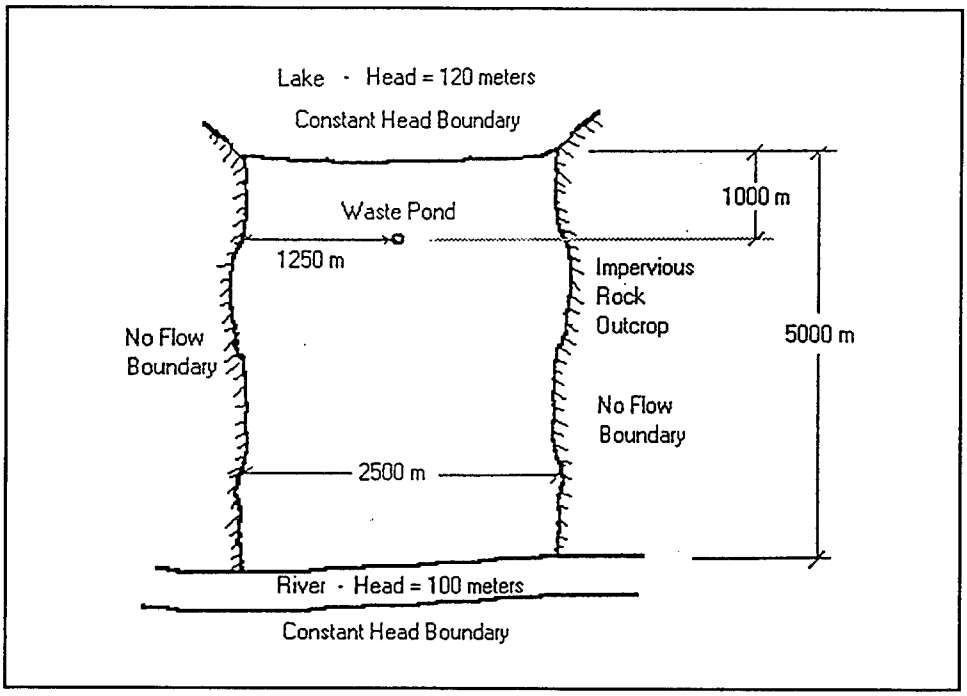

Figure 19. Areal view of WES Example Problem 1

Table 6
Aquifer Properties for WES Example Problem 1

Hydraulic conductivity	10 m/day
Porosity	0.35
Specific yield	0.30
Dispersivity (direction) x y z	 10 m 1 m 1 m

4 Models Description

Saturated Flow and/or Transport Models

MOC

The U.S. Geological Survey Method of Characteristic (USGS-MOC or MOC) is an areal, two-dimensional, numerical model for flow and transport (F&T) in saturated, porous media. Media properties, flow and transport options, model features, and numerical methods include the following:

- *Flow Conditions*: The model simulates horizontal, two-dimensional (2-D) (x-y plane) F&T in an aquifer. Vertical F&T other than leakage from confining units is assumed negligible. Steady-state or transient solutions may be simulated for confined aquifers; steady-state solutions may be obtained for unconfined aquifers (i.e., distribution of saturated thicknesses is established and constant). Water is slightly compressible; storativity is required for transient simulations. Flow is assumed unaffected by spatial variation in water density or viscosity (i.e., the model assumes low solute concentrations and isothermal conditions).

- *Porous Media Conditions*: Only saturated F&T problems are simulated. The medium may be confined or unconfined (if steady-state saturated thickness is established). Porosity is constant and uniform. Block-scale, spatial variations in aquifer thickness, transmissivity, initial heads, and solute concentrations are accommodated. Permeability is constant and may be anisotropic as defined with a single K_{xx}/K_{yy} ratio (ANFCTR).

- *Initial Conditions*: Spatially variable, initial estimates may be defined for head and/or concentrations.

- *Boundary Conditions*: All peripheral cells are modeled as no-flow boundaries. No-flow cells ($T = 0$) may also be defined for interior cells. Constant-head cells may be defined. Constant-flux cells may be defined for diffusive recharge (leakage) or well flow (injection or withdrawal). Any number of wells may be defined.

- *Transport Processes*: USGS-MOC solves an advection-dispersion equation (see below). Advection is solved based on velocity vectors calculated from head distributions on the finite-difference grid. *Hydrodynamic dispersion* is modeled as dependent on dispersivity (longitudinal and transverse) and seepage velocity. Adsorption is modeled using a retardation factor approach(see Appendix B). Retardation factors may be calculated for linear, Freundlich, or Langmuir equilibrium isotherms or for ion exchange (mono- or di-valent) reactions. *Decay* is modeled as a first-order loss (or gain if $\lambda < 0$) and is assumed to affect solute and adsorbate equally. Decoupling of flow from solute concentration precludes density or viscosity effects on flow, i.e., solute concentrations must be low.

- *Miscellaneous Features*: Multiple pumping periods allow for limited changes in flow conditions (well pumping rates and/or concentrations).

- *Mass Balance Calculations*: Global mass balances for water and solute are calculated at each output of concentration distribution data.

Input/Output Parameters. Any consistent units (English or metric) may be used, though standard output is in English units. User may specify up to five observation cells. The user may regulate the type and frequency of output to a limited degree; generally, the output file is quite large. Preprocessor and Postprocessor are available for MOC (e.g., IGWMC's PREMOC, Geraghty & Miller's ModelCad-386 and MOC2SURF). In this evaluation, ModelCad-386 was used to generate part of the input data.

Equations. The USGS-MOC simulates transient, areal flow of a homogeneous, compressible fluid, in Cartesian coordinates, as described by (Konikow and Bredehoeft 1978):

$$\frac{\partial}{\partial x_i}\left(T_{i,j}\frac{\partial h}{\partial x_j}\right) = S\frac{\partial h}{\partial t} + Q(x,y,t) - \frac{K_2}{m}(H_s - h) \qquad (21)$$

Storage *Injection or withdrawal* *Leakance*

where

$T_{i,j}$ = transmissivity tensor $[L^2T^{-1}]$

h = hydraulic head $[L]$

S = storage coefficient [-]

t = time

$Q_{i,j}$ = well flow rate (+ ≡ injection, – ≡ withdrawal)

K_Z = vertical hydraulic conductivity $[L\,T^{-1}]$ of confining layer

m = thickness of confining layer

H_S = head in source bed

The transport equation solved is as follows (Goode and Konikow 1989):

$$\frac{dC}{dt} + \frac{\rho_b K_d}{\varepsilon}\frac{dC}{dt} = R_f \frac{dc}{dt} =$$

$$\frac{1}{b}\frac{\partial}{\partial x_i}\left(b D_{i,j}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} + \frac{W(C-C')}{\varepsilon b} - \lambda C - \frac{\rho_b}{\varepsilon}\lambda S \quad (22)$$

Dispersion *Advection* *Sink or Source* *Decay* *Sorption or Ion Exchange*

where

C = solute concentration

ρ_b = bulk density [$M\,L^{-3}$]

ε = porosity [–]

K_d = partitioning coefficient [$L^3\,M^{-1}$]

R_f = retardation factor ($\equiv 1 + (\rho_b K_d) / \varepsilon$)

λ = first-order decay coefficient [T^{-1}]

b = aquifer saturated thickness L

S = adsorbate concentration [$M_C\,M_b^{-1}$]

Hydrodynamic dispersion is dependent on flow velocity and dispersivities. Retardation is applied to particle velocities based on grid-averaged concentrations. The model assumes the following:

- Darcy's Law is applicable.
- Porosity and conductivity are constant over time.
- Molecular diffusion is negligible.
- Vertical variation in head and concentration is negligible.

Numerical methods for flow. Head distribution is solved with a block-centered, finite-difference scheme. Grid spacing is regular and rectangular (constant Δx and Δy). The maximum grid size may be limited by the program's compiled version used, but the source code is easily modified. The flow equations are solved with an Alternating Direction - Implicit Procedure (ADIP). Particle velocities are calculated by bilinear interpolation from nodal solutions.

Numerical methods for transport. Single-solute advective transport is simulated by the MOC using a particle-tracking technique. The user specifies the number of particles per cell (4, 5, 8, 9, or 16). The 1989 version introduced an option for a transport subgrid. The compiled version allows a 40 by 40 grid for flow with an option to designate a 20 by 20 subgrid for transport. Source terms, divergence, and velocity-dependent, hydrodynamic dispersion are simulated with a two-step, explicit finite-difference method.

Evaluation. Performance of USGS-MOC is evaluated by application to three sets of problems: (a) four, 2-D scenarios proposed by the code developers and included in the original documentation—three from Konikow and Bredehoeft (1978), one from Goode and Konikow (1989); (b) three scenarios for which analytical solutions are available—transport of a solute continuous point-source, a slug release, and radial transport from an injection well; and (c) and artificial scenario (WES Example 1).

Examples. USGS-MOC was able to solve all four of the 2-D benchmarks included in the documentation. These benchmarks were designed to demonstrate various features and capabilities of the model. Analytical solutions are not available for these scenarios.

Problems with analytical solutions. Three test cases, described in Chapter 3, for which analytical solutions are available were simulated. Analytical solutions included in the SOLUTE package (Beljin 1991) are adopted as the reference solutions for the following:

a. Dispersal from a continuous point source: steady-state flow in an infinite, uniform, homogeneous, confined aquifer via a fully penetrating well, at a recharge rate negligible relative to regional flow; the PLUME2D - Point Source analytical solution is used.

b. Dispersal of a solute slug released instantaneous into an infinite, uniform, homogeneous, confined aquifer; simulated with the PLUME2D - Slug Source.

c. Continuous, radial transport into a planar, confined aquifer of infinite extent; the RADIAL analytical solution is employed.

Continuous point-source transport. A constant concentration cell is imposed at the upgradient margin of a steady-state flow field to simulate this problem with USGS-MOC. The model performed well, closely predicting concentrations and arrival times. Mass balance errors were small and improved with time (3.6 percent at Day 500; <1 percent for times ≥ 1,000 days). The solute was modeled as a conservative tracer.

Slug transport. An initial concentration assigned to a cell at time zero is allowed to disperse in a uniform, steady-state flow field. USGS-MOC tended to overestimate the peak concentration at short times when concentration gradients were the most steep. Agreement with the analytical solution improved as the solute slug dispersed downgradient. Conservative behavior was assumed for the solute. Mass balance errors were acceptable, all less than 1.1 percent.

Radial transport. Simulation of radial transport with a model operating in Cartesian coordinates is a severe and perhaps inappropriate test. USGS-MOC does not yet include an option for radial coordinates. For the present purpose, radial transport is simulated with an unmodified code using a fully penetrating well to inject a conservative solute into a confined aquifer with no regional head gradient. Head is fixed at a single value in an octagonal pattern (as an approximation to circular) around the injection

well node. At high longitudinal dispersivity (α_L = 0.984 ft)[1] and negligible transverse dispersivity (α_T = 0.0098 ft), the model predicts impeded transport along grid axes relative to paths at a 45-deg angle to grid axes. The concentration profile indicated by the diagonal trend closely approximates the analytical solution, whereas the trend along an axis greatly underestimates transport.

The origin of this pronounced grid effect is uncertain. Steady-state head distribution, and therefore radial velocities, are axisymmetric about the center of the injection well cell. Setting transverse dispersivity equal to the longitudinal dispersivity in MOC tends to decrease the disparity between diagonal and axial flow paths, at least at longer travel times. The shape of the model concentration profile mimics the analytical solution, but is lagged by a small distance (approximately 1 to 2 ft at 40 days). This disparity is likely the result of the difference between the dimension of the finite-difference cell and the well-bore diameter in the analytical solution (apparently fixed at 0.25 units in RADIAL). In MOC, the injected solute is dispersed uniformly over the volume of the finite-difference cell, which effectively disperses the solute and does not simulate the high radial flow velocity near the well bore predicted with the analytical solution.

Discretizing to the scale of a well diameter is impractical, but would probably show better agreement between the model and analytical solution. Mass balance errors were less than 8 percent, considerably greater than the other scenarios. Konikow and Bredehoeft (1978) compare MOC with an analytical solution for radial flow, but only after modifications to the code, including an analytical expression to calculate a radial flow velocity, which are not part of the standard code. If a low regional gradient is imposed, the grid effect is diminished.

Hypothetical scenario. USGS-MOC was applied to a simple artificial scenario that involves the leakage of solute from a wastewater lagoon into an unconfined aquifer. Regional flow gradient and head boundary conditions are set by surface water elevations defined as steady (120 and 100 m). Lateral boundaries are defined as no-flow (impermeable rocks). The saturated thickness above a horizontal, impermeable datum (70 m) is assumed to decrease linearly from 50 upgradient to 30 m over the 5,000-m length of the flow field.

Application of USGS-MOC to a steady-state, unconfined flow and transport problem requires a preliminary run of the model to evaluate the effects of the recharge from the lagoon on saturated thickness (piezometric surface elevation minus horizontal datum) below the pond. The effect is minor due to low recharge rates, but is simulated. With USGS-MOC this requires the tedious transfer of formatted head outputs to the next input file and calculation of a spatially variable transmissivity field (e.g., with a spreadsheet). The code could be modified to generate output in the proper format for insertion into the next simulation input file, but this is not a standard feature. Solute loading is modeled as a fully penetrating,

[1] A table of factors for converting non-SI units of measurement to SI units is presented on page xi.

injection well, given a flow rate and concentration. Results appear reasonable. No analytical solution is available for comparison. This benchmark is intended for intercode comparisons.

Summary. The USGS-MOC code is in the public domain; therefore, source codes are available at nominal cost. The code is fairly mature and has a relatively large user community. Many updates and new versions of MOC have been developed since 1978. The 1989 version (Goode and Konikow 1989) introduced nonconservative behavior including adsorption and first-order decay. MOC has been adapted to simulate oxygen-limited, aerobic biodegradation (BIOPLUME-II; Rifai et al. 1987), two-constituent, variable density transport (MOCDENSE; Sanford and Konikow 1985), a simplified, nonaqueous phase flow model (Hossain and Corapcioglu 1985) and others. Further enhancements are likely.

MOC assets in remediation simulation are numerous. The method of characteristics is well suited for solving advection-dominated transport equations (hyperbolic), which are commonly encountered in remediation systems. MOC reduces numerical dispersion, relative to traditional finite-difference or finite-element methods, by not propagating such erroneous dispersion throughout the simulation. Thus, steep concentration gradients may retain their integrity.

As stated before, MOC is a mature, well-established, well-documented code and is among the most commonly used numerical models for remediation design.

There are significant limitations in utilizing MOC for remediation. Some of the more serious are as follows:

- Standard MOC methods are intrinsically not mass conservative, particularly at early times of solute injection. Mass balance errors for solute typically are less than 5 to 10 percent.
- MOC uses more particles than some other MOC-based codes; e.g., 4 to 16 particles in each transport grid cell, regardless of the presence of solute. The transport subgrid was introduced to address this inefficiency.
- Imposing a truly fixed concentration at a cell is not a standard option. Code modification would be required, including reworking the mass balance calculations.
- The MOC does not as yet have an option for radial transport. The Cartesian coordinate system of the standard code does not handle radial transport well, particularly at short times or low dispersivity.
- The model should not be used for cases in which both a nonlinear isotherm and no dispersion are invoked (Goode and Konikow 1989; p.17); smooth concentration gradients are required to avoid complications with the method of calculating retardation factors (based on cell-averaged concentrations, not individual particles).
- Decay for solute and adsorbate may be identical for radionuclides, but not typical for most organic solutes subject to biotransformation or abiotic reactions.

MODFLOW

MODFLOW is a three-dimensional numerical model for flow through saturated, porous media. Medium properties, flow options, model features, and numerical methods include the following:

- *Flow Conditions*: MODFLOW solves for saturated, isothermal, three-dimensional flow through confined, unconfined, or convertible (confined/unconfined) aquifers. Flow solutions may be steady state or time dependent. Each simulation may contain multiple "stress periods" between which the sources and sinks (e.g., wells) and the boundary conditions may change strength. Variable fluid density and viscosity are not considered.

- *Porous Media Conditions*: The hydraulic conductivity (transmissivity for confined aquifers) must be specified for each computational cell and may not change with time. For time-dependent simulation, the primary storage coefficient also must be specified for every computational cell. In an unconfined layer, this coefficient is the specific yield; for all other layers, it is the specific storage coefficient times the layer thickness. For confined/unconfined layers, the specific yield is entered as the secondary storage coefficient and the model selects the appropriate storage coefficient. The model can simulate anisotropic media, but assumes that the coordinate directions are aligned with the principal axes of the medium's conductivity. In this manner, the full conductivity tensor is not needed; only the primary-direction hydraulic conductivities are required. This assumption is appropriate for media with generally parallel layers and is reasonable when the deviation from this assumed parallel structure is not great (e.g., such as discontinuous, or highly nonparallel geologic formations). Anisotropy is simulated by introducing a single ratio of K_{xx}/K_{yy} for each layer and in the separate specification of the vertical conductance for each cell.

- *Initial Conditions*: Initial values for head may be specified within the input file, read from an external file, or read from a file written by a previous simulation with this model.

- *Boundary Conditions*: Each computational cell must be declared as either inactive (no flow), as constant head, or as variable head. One equation is solved for every variable head cell in the field. Other than a general head boundary, most boundary condition implementation is transparent to the user and is performed automatically when the user selects hydrologic stress packages. For example, the river package requires that cells contain a specified head, and the recharge package includes a specified flux.

- *Hydrologic Stresses*: The model has specific packages to deal with wells, recharge, drains, rivers, gaining/losing streams, and evapotranspiration.

- *Transport Processes*: None. The model solves only for heads and cell-by-cell flow. Transport must be simulated with a separate model using the MODFLOW heads and flows.

- *Miscellaneous Features*: The model is capable of running from a "hot-start." That means the model can read heads from a previous simulation's output and effectively continue that simulation.

- *Mass Balance Calculations*: A mass balance of water is determined by the model. The mass balance error, computed by subtracting the total sinks from the total sources, is normally very small (a few percent or less). Some problems have been noted using General Head Boundary Conditions (Anderson and Woessner 1992).

- *Discretization*:
  Space: The model permits either quasi or fully three-dimensional application. If confining layers are lumped into the vertical conductance and not explicitly discretized, the medium is represented as a series of two-dimensional aquifers with leakage. If all layers are discretely described, three-dimensional flow fields can be obtained. Cells must be rectangular in plan view, but can vary in thickness to comply with mildly nonparallel geologic formations. These layer thickness variations are not implemented in the model directly but are introduced by varying the input medium properties such as transmissivity. The extended memory version of the model uses semidynamic storage allocation, meaning there is no preset limitation on the number of computational cells in the domain. All model variables are stored in a large, one-dimensional array. The number of cells that can be simulated depends on the other options selected in the simulation. A rule of thumb is provided by McDonald and Harbaugh (1988) stating that the total storage requirements are usually 10 to 20 times the number of cells. In the IGWMC version, about 36,000 total cells can be simulated (e.g., 60 rows, by 60 columns, by 10 layers). With an appropriate FORTRAN compiler, the dimension of this array can be changed and the model recompiled.
  Time: As stated earlier, MODFLOW is an implicit model, meaning that the equations for every cell are solved simultaneously. This process removes the stability constraints in selecting the size of time steps. However, very large time steps should be avoided in an evolving flow field because the numerical approximation of the time derivative creates error that is proportional to the time step size. In general, time discretization for implicit models is governed more by the desired output frequency and the timing of changes in external stresses. MODFLOW solves the set of simultaneous, linear equations by iteration. An initial guess for the head field is provided to the solver. The equations are solved and the heads are adjusted until the head change is negligible over an iteration. Three iterative solvers (the strongly implicit procedure, slice-successive overrelaxation, and a preconditioned conjugate gradient solver) are provided. For unconfined flow, the equation is linearized by using the heads from the prior iteration to compute transmissivities for the present iteration.

Input/output parameters. Any consistent units (English or metric) may be used. The input units are for printout only and do not affect the calculations. The user has extensive control over the quantity and appearance of the model output. Preprocessing and postprocessing programs are available to assist with model setup and data visualization. MODFLOW is one of the models included in the GMS Version 1.0.

Equations. The governing partial differential equation used in MODFLOW is a combination of Darcy's Law and a statement of mass conservation that gives

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W = S_s\frac{\partial h}{\partial t} \qquad (23)$$

where

K_{xx}, K_{yy}, and K_{zz} = primary direction hydraulic conductivities $[LT^{-1}]$ for the x, y, and z coordinate directions

h = potentiometric head $[L]$

W = external stress (source/sink) term $[T^{-1}]$

S_s = specific storage $[L^{-1}]$

Within the above equations, the model has assumed the following:

- Darcy's Law is applicable.
- Conductivities (or transmissivities) and storage coefficients may vary spatially, but are constant in time.
- The coordinate axes are aligned with the principal directions of flow. In this manner, the conductivity tensor reduces to a diagonal matrix containing only K_{xx}, K_{yy}, and K_{zz}.

In the limited space available for this brief model description, the many MODFLOW packages and the equations they use cannot be discussed individually. In addition to those packages described in the model's 1988 documentation, other packages are becoming standard with most MODFLOW distributions including the following:

- BCF2 - (McDonald et al. 1991) permits rewetting of dry cells.
- STR1 - (Prudic 1989) stream routing in concert with groundwater modeling.
- PCG2 - (Hill 1990) preconditioned conjugate gradient solution procedure.

Additional packages are available. Examples include the following:

- A Horizontal Flow Barrier Package for the simulation of slurry walls.
- An updated Block Centered Flow Package (3) that computes improved interblock transmissivities for unconfined flow.

Numerical methods. A block-centered finite difference method is used. With this method, a node is defined at the center of each finite difference cell. The modeled variable (head) is computed at the nodal location. Geologic and hydrologic parameters are known at the nodal locations and are assumed to be constant within the confines of each finite difference cell. Hydraulic conductivities are known at the cell centers, but are needed at each of the cell faces for computation of flux through that face. Cell-face hydraulic conductivities are approximated using a harmonic mean of the

conductivities in the two adjoining cells. Vertical conductivity between layers is handled slightly differently. Instead of specifying a vertical hydraulic conductivity value for each cell, vertical conductance is specified at the cell faces between the layers. Vertical conductance is the effective vertical hydraulic conductivity for the face divided by the vertical distance between the nodes in the adjoining cells.

Head in a cell is computed by equating the sum of the face fluxes and any external sources or sinks to the change in storage for that cell over that time step. The time derivative is approximated by a first-order, backward difference method, which means that this is an implicit scheme.

Evaluation. In this phase of the model evaluation, the MODFLOW model is compared with two sets of problems: (a) five example problems provided with the original model distribution (McDonald and Harbaugh 1988; MODFLOW course notes); and (b) two scenarios for which analytical or approximate analytical solutions are available.

Examples. MODFLOW was able to solve all five of the benchmarks provided and documented with the code. These benchmarks were designed to demonstrate various features and capabilities of the model. Analytical solutions are not available for these scenarios. The model results appear reasonable and agree with the documented simulation results.

Synthetic scenarios with analytical solutions. Two synthetic benchmarks are defined for which analytical or approximately analytical solutions are available. These benchmarks were designed to test some of the fundamental capabilities of the flow model. The media are assumed homogeneous.

a. Steady-state and long-time transient flow between two, parallel ditches in an unconfined aquifer with uniform recharge.

b. Time-dependent solution of multiple wells in a bounded, confined aquifer.

Flow between two ditches with uniform recharge. The flow between two infinitely long, parallel ditches with different, fixed heads was examined both with and without uniform recharge. The analytical solution for the case without recharge is a simple parabola. With recharge, the analytical solution is obtained by superposing the parabolic solution and the ellipse that describes recharge between two ditches assuming horizontal groundwater flow (for example, McWhorter and Sunada 1977). MODFLOW reproduced the two curves almost exactly. Errors were less than 0.01 m in a 100+ m thick aquifer. The same problem was simulated as a long-time transient solution in MODFLOW. The model reached almost exactly the same answers as the steady-state solution.

Multiple wells in a bounded domain. Time-dependent flow in a confined, bounded, 2-D (planar) square domain was examined in the presence of two recharge wells and one pumping well. The boundaries consisted of two adjacent impermeable boundaries and two adjacent constant head boundaries. The analytical solution can be obtained by a method of images solution for the wells. The problem is time dependent, so the

Theis solution provides an analytical solution for confined flow. Again, the model performed reasonably well. Wells and other rapidly converging/diverging flows provide a severe challenge to Cartesian-based numerical techniques. Errors in head were less than 0.5 m for all comparisons more than two grid cells away from a well. Exactly at the well positions, the differences are larger because the discrete approximation predicts a spatially average drawdown, while the analytical solution provides point values. Maximum piezometric head change in the domain from the flat initial condition was about 55 m. This simulation took about 20 to 30 sec to execute.

Summary. The USGS MODFLOW model is in the public domain. Therefore, it can be obtained in original form for a nominal cost ($40 from the USGS including documentation). The model basis has received significant public scrutiny and has been widely applied. MODLOW's current popularity suggests that the model will be well maintained and frequently upgraded.

Training is also easily found. The International Ground Water Modeling Center and many others offer training in the use of MODFLOW.

MODFLOW's assets in remediation modeling relate to the model's versatility, third-party support, and code's maturity. The model is very flexible and can accommodate a wide variety of hydrologic and geologic conditions. The model is evolving rapidly as evidenced by the recent addition of many packages and interfaces. MODFLOW contains packages that implement hydrologic boundary conditions automatically and transparently to the user. This is superior to models that require users to know when and how to numerically implement a boundary condition.

Despite the way it is sometimes used, MODFLOW is not the answer for all groundwater contamination problems and, in particular, remediation simulation. Some of the deficiencies are as follows:

- It cannot realistically simulate coupled flow and transport problems, contamination by nonaqueous phase liquids, nonisothermal conditions, etc.
- The use of a diagonal conductivity matrix rather than the full conductivity tensor is a restriction. For many natural systems, the assumption that there are three primary directions of flow and that the grid can be oriented, such that these follow the x, y,and z directions, is valid. However, the assumption may be less reasonable during remediation when the flow field will be subjected to non-natural forcing.
- The grid-generation system is not nearly as flexible as unstructured or boundary-fitted structured gridding. The limitation arises when the user wishes to have increased resolution in a localized area. With MODFLOW, if Row 3 is 10 m wide, it is 10 m wide in the area of real interest and 2 miles away at the river. This problem is most pronounced when the model domain must be extended beyond the local area of interest to make use of known hydrologic boundary conditions.

- Data input and output are not straightforward, especially for new users. Text-based preprocessors help some. Graphical preprocessors like MODELCAD[386] help more but are not comprehensive. This program essentially has added graphics to the standard MODFLOW input rather than accessing databases and establishing cell information by interpolation automatically. Editing grids and modifying existing files graphically is still a bit cumbersome. Once an application has been set up, making changes to the input files is best performed with a text editor and the MODFLOW manual. Some of the limitations of existing preprocessors are overcome by the GMS Version 1.0.
- Strongly converging and diverging flows, like those near a well, cause difficulties for the Cartesian-based models. MODFLOW is no exception.

Overall, MODFLOW is recommended for groundwater flow problems that do not involve temperature variation, density variation (e.g., salt water and fresh water), unsaturated flow or nonaqueous phase contaminants, fractures, highly heterogeneous porous media, or geometries that cannot be reasonably represented by many, small rectangles. For transport problems, MODFLOW can be used with a transport model such as MODPATH for advection only or, more appropriately, with MT3D for advection, dispersion, and reactions. The MT3D-compatible version of the model, MODFLOW/mt, is probably a wise choice for use with MT3D because the linkages between the codes have already been performed.

MT3D

MT3D is a three-dimensional numerical model that simulates transport in saturated porous media. Media properties, transport options, model features, and numerical methods include the following:

- *Flow Conditions*: The MT3D model does not solve the equations for flow through porous media. Rather, this model relies on head distributions, Darcy velocities, and locations and flow rates of sources and sinks to be provided externally (normally from a groundwater flow model). Flow solutions provided to the MT3D model may be steady state or time dependent and may contain multiple "stress periods" between which the sources and sinks may change strength and location. Because of the decoupling of the flow and transport solutions, the flow is necessarily assumed to be unaffected by the solute concentration.
- *Porous Media Conditions*: This model assumes that the medium is saturated. The medium layers may be confined, unconfined, or convertible. Porosity must be specified for each computational cell and may not change with time. Values of other medium properties, such as hydraulic conductivity, are not relevant to the MT3D transport model because their effects are imbedded within the solution to the flow equations. The model requires that spatially variable layer thicknesses and top elevations be provided.

- *Initial and Boundary Conditions*: Initial solute concentrations must be specified for each computational cell. Each computational cell must be declared as either inactive for transport, as a constant concentration cell, or as active for transport (variable concentration). Besides constant concentration cells, the model also permits specified concentration gradients or a combination of specified concentration and gradient. An example concentration gradient boundary condition is an impermeable boundary for which the dispersive contaminant flux (and therefore concentration gradient) is known to be zero. Most boundary conditions are selected indirectly by the user through application of the transport packages.

- *Transport Processes*: The model simulates advection, dispersion, sources/sinks, and reactions. Advection is solved based on seepage velocities computed by dividing the Darcy flux (from the fixed-grid flow solution) by the porosity. Hydrodynamic dispersion is simulated using longitudinal and two transverse dispersivities, seepage velocities, and molecular diffusion. Sources and sinks can take many forms including wells, drains, recharge, evapotranspiration, rivers, and general-head-dependent boundary cells. Reaction includes both adsorption and first-order decay or biodegradation. Adsorption assumes local equilibrium and may be approximated by linear, Freundlich, or Langmuir isotherms. Decay (or biodegradation) is irreversible. The rates of loss (or gain) of contaminant may be different for the solute and the adsorbate. The adsorption and reaction parameters may not vary with time or in space. A single value for each parameter applies everywhere in the domain for the entire simulation.

- *Miscellaneous Features*: The model is capable of running from a "hot-start." That means the model can read ending-state information from a previous simulation to continue that simulation. Long simulations can be broken into smaller ones to avoid the creation of very large output files.

- *Mass Balance Calculations*: Global mass balance of contaminant is computed by the model and is relied upon often to assess the worth of model results. The model output includes a breakdown of the mass introduced and removed from the domain by each of several means including constant concentration cells, wells, recharge, decay, and adsorbed and solute mass storage.

- *Discretization*:
  Space: Spatial discretization is handled in the same manner as in the MODFLOW model. Cells must be rectangular in plan view, but can vary in thickness to comply with geologic formations. There is no preset limit on the number of computational cells in the domain. Rather, it is a function of the memory available on the computer. The source code uses two large one-dimensional arrays to store values for all the model variables. In this manner, the limitation on grid dimensions depends on the options chosen (number of particles, etc). The executable file provided in the package uses fully dynamic memory allocation, which accesses memory at run-time. With this option, the program can run any problem that will fit in the available

RAM. If run in Windows, the program can use space on the hard disk as virtual memory.

Time: Unlike implicit flow models such as MODFLOW, MT3D is explicit and has restrictions on the size of its time steps. It projects a future value of concentration for a cell based on present information. The model computes the step size limitations for advection, sources, dispersion, and reaction and chooses the most restrictive step size. If the user-specified step size is smaller than that computed by the model, the user-specified size is applied. The step size is used to subdivide the flow time steps that are read as part of the flow solution. Therefore, there may be many transport steps within a single flow step. Time advancement is accomplished by either a first-order Euler method, a fourth-order Runge-Kutta method, or a combination of both methods. The combined method uses the more accurate fourth-order scheme where it is needed (near sources and sinks) and the more efficient first-order scheme away from strongly converging/ diverging flows.

Input/output parameters. Any consistent units (English or metric) may be used. The units specifications in the input file are for output only and do not affect the calculations. The user has extensive control over the quantity and appearance of the model output. The size of the output may range from a few pages to a file quite large. Limited preprocessing and post-processing capabilities are discussed below.

Equations. The governing partial differential equation used in MT3D is the traditional advection-dispersion equation, which describes the changes in concentration due to dispersion, advection, sources and sinks, and reactions (Zheng 1992)

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i C) + \frac{q_s}{\theta}C_s + \sum_{k=1}^{n} R_k \qquad (24)$$

dispersion *advection* *source* *reaction*

where

D_{ij} = hydrodynamic dispersion coefficient $[L^2T^{-1}]$

C = concentration $[ML^{-3}]$

v_i = seepage velocity $[LT^{-1}]$

qs = source/sink flow rate $[L^3T^{-1}]$

θ = porosity [-]

C_s = source concentration $[ML^{-3}]$

R_k = reaction rate $[ML^{-3}T^{-1}]$

The dispersion coefficient is a second rank tensor. The *xx* component of the dispersion coefficient tensor is given by

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_{TH} \frac{v_y^2}{|v|} + \alpha_{TV} \frac{v_z^2}{|v|} + D^* \tag{25}$$

where

α_L = longitudinal dispersivity [L]

v = magnitude of the velocity vector [LT^{-1}]

α_{TH} = horizontal transverse dispersivity [L]

α_{TV} = vertical transverse dispersivity [L]

D^* = molecular diffusion [L^2T^{-1}]

The general form of the reaction term in the transport equation is

$$\sum_{k=1}^{n} R_k = \frac{\rho_b}{\theta} \frac{\partial C'}{\partial t} - \left(\lambda_1 C + \lambda_2 \frac{\rho_b}{\theta} C' \right) \tag{26}$$

adsorption *decay*

where

C' = adsorbed concentration [ML^{-3}]

ρ_b = bulk density of the medium [ML^{-3}]

λ_1 = decay or biodegradation rate for solute [T^{-1}]

λ_2 = rate for adsorbate [T^{-1}]

The amount of contaminant adsorbed to the medium is assumed to be a function of the dissolved concentration only. Based on the type of isotherm chosen (linear, Freundlich, or Langmuir) the model computes a retardation factor due to adsorption. Reactions are applied based on grid-averaged concentrations. Within the above equations, the model has assumed the following:

- Darcy's Law is applicable.
- Porosities, dispersivities, and reaction parameters are constant in time.

Numerical methods. MT3D uses a mixed Eulerian-Lagrangian solution scheme. Four options are provided for the simulation of the advection component of transport. These options are three Lagrangian-based, particle-tracking methods (MOC, MMOC, and HMOC) and a fixed-grid-based (Eulerian), block-centered, upwind finite-difference scheme. The MOC (method-of-characteristics) technique projects the future location of particles advected by the seepage velocities and produces very little numerical dispersion. The MMOC (modified-method-of-characteristics) tracks a single, cell-centered particle backward in time using the seepage velocities

to determine its location at the beginning of the time step. MMOC is more efficient than MOC but contains some numerical dispersion from the interpolation process. The hybrid-method-of-characteristics (HMOC) technique takes advantage of the strengths of each of these methods by using MOC near large concentration gradients and MMOC elsewhere in the field. Although very dispersive and not routinely recommended, upwind finite differences are included as an option for the advection term because, unlike particle schemes, they are mass conserving and computationally efficient. Dispersion, sources and sinks, and reaction processes are simulated by an Eulerian, block-centered, explicit finite-difference method.

Evaluation. Performance of the MT3D model is evaluated by comparison to two sets of problems: (a) ten example problems provided with the model (Zheng 1992), and (b) three scenarios for which analytical solutions are available.

Examples. MT3D is packaged with 10 example problems that range from model comparison against analytical solutions to sample applications in multidimensional heterogeneous media. The example problems demonstrate various features and capabilities of the model. The model was able to execute all 10 benchmarks provided with the code. The results compare well with analytical solutions where available and appear reasonable for problems with no analytical solutions.

Problems with analytical solutions. Three synthetic benchmarks are defined for which analytical solutions are available. Analytical solutions included in the SOLUTE package (Beljin 1991) are adopted as the reference solutions for the following:

a. A concentration plume emanating from a continuous point source in a uniform two-dimensional flow field.

b. A concentration plume produced by a slug point source in a uniform, two-dimensional flow field.

c. A concentration plume produced by radial transport from a fully penetrating recharge well in an infinite, planar aquifer.

Continuous source in a uniform flow. Contamination was introduced at a constant rate through a fully penetrating well in a steady-state flow. The medium is an infinite, homogeneous, confined aquifer of constant thickness, and the recharge rate is negligible relative to regional flow. The PLUME2D - Point Source analytical solution is used. Comparisons are made with and without retardation and decay. The model performed very well in predicting both the magnitude and arrival time of the contaminant when modeled as a conservative tracer. Mass balance errors were acceptably small, ranging from 1 to 5 percent. Likewise, the MT3D concentrations predicted with retardation and decay matched closely with the analytical solutions. Again the mass balance errors were acceptable.

Slug source in a uniform flow. Contamination was introduced in the initial condition to the model and allowed to disperse in a uniform, steady-state flow field. No decay or adsorption was simulated. MT3D matched the speed of the peak and approximated the amplitude very well.

The model tended to slightly overpredict the amplitude of the peak at early times. Some wiggles in the predicted peak can be seen, but are not considered significant. Overall, the mass balance error was an acceptable 2.5 percent at 16 days.

Continuous source in a steady, radial flow. MT3D is not capable of discretizing a domain in radial coordinates. Therefore, a radial transport problem presents a significant challenge. A fully penetrating injection well was placed in an otherwise stagnant, confined, infinite, homogeneous medium. The well injects at a constant rate and establishes a steady-state flow field. The contaminant was introduced into the well at a constant rate of 1.0 ppm. The analytical solution was provided by the RADIAL program within the SOLUTE package. The MODFLOW/mt flow solution was generated in a finite domain by computing, by hand, the boundary values of head that would produce the desired flow and installing these as constant heads in the model. This flow field was then used for the MT3D simulations. The results show a generally circular spreading of the contaminant. There is no visible difference between the contaminant advancement along a gridline and diagonal to the gridlines. Comparison with analytical results show a good agreement for all three values of longitudinal dispersivity tested. The mass balance errors for these simulations ranged from about 6.5 percent at 20 days to less than 3 percent at 40 days.

Summary. MT3D is a proprietary code that is the property of Dr. Chunmiao Zheng and S. S. Papadopulos and Associates, Inc. It is available for $450. The EPA's Robert S. Kerr Environmental Research Laboratory distributes MT3D Version 1.2 through CSMoS, but the model is relatively new and has not received the same degree of public scrutiny as many of the USGS models. The model's roots date back only about 6 years (Zheng 1988). The model has been in a form similar to today's version for only about 4 years. However, its current popularity and ties to the immensely popular MODFLOW program suggest that the model probably will be maintained and upgraded.

The developer of the program has moved recently from SSP&A to the University of Alabama. SSP&A insist that they will continue to support and distribute the model and that they will continue to work with Dr. Zheng. Although upgrades are promised, his departure makes future upgrades to the program and to the MODFLOW/mt flow solver slightly less definite.

Support for the model goes through SSP&A or Dr. Zheng. As of 1993, with the purchase of MT3D, users are entitled to 20 min of telephone support in the first year, the right to purchase, by contract, additional telephone support at about $2 per minute and notification of the availability of upgrades via a newsletter for registered users.

MT3D assets for remediation simulation are many. The model simulates many important transport processes including advection, dispersion, different decay rates for the solute and the adsorbed contaminant, and sorption. This makes MT3D vastly superior to pathline codes that only track the advective component of transport.

The particle-based Lagrangian approach is superior to coarse-grid Eulerian schemes for simulating advection-dominated problems. Steep

concentration gradients can be simulated without smearing of peaks. The model can accept steady-state or transient-flow solutions. This is a very important attribute for remediation. It is unlikely that the hydrologic stresses will remain constant over the life of a remediation project.

The developer considered computational speed and memory requirements when building the model. Several examples are readily available. Regions of the flow domain that will not experience contamination can be declared inactive for transport computations. Also, particles for the MOC solution are allocated dynamically. In this manner, particles are only introduced where contamination exists. The use of MMOC away from concentration gradients is driven by computational speed and memory considerations. This attention to detail makes the MT3D model well suited to microcomputer application—even for large problems.

MT3D limitations in remediation modeling stems mostly from inherent problems with MOC-type methods in conserving mass. Mass conservation is difficult to ensure with particle-based codes. Mass balance errors less than 10 percent are considered acceptable.

There are very many options in the numerical implementation of the advection process. The user is asked (permitted) to select planes of particle introduction, maximum and minimum numbers of particles, critical concentration gradients, etc., that have no meaning for someone unfamiliar with the inner workings of a particle-tracking program. Manipulation of these model parameters is sometimes necessary to achieve a stable, physically meaningful answer with an acceptable mass balance error.

Unlike some of the more complicated transport codes, this model is limited to small concentrations. The transport code is completely decoupled from the flow solution. This precludes the simulation of flows that are affected by contaminant concentrations (density-dependent problems).

Overall, for a saturated medium in which the flow and transport solutions can be decoupled (density variations are small), the use of MODFLOW/mt with MT3D is highly recommended. The models are sufficiently simple that set up, and modification can be performed in a reasonable time frame. However, when combined, these models have most capabilities required for routine flow and transport modeling. MT3D will be included in the GMS in late FY95.

PLASM

The Prickett-Lonnquist Aquifer Simulation Model (PLASM) is a groundwater flow simulation model. The model was developed for the Illinois State Water Survey (Prickett and Lonnquist 1971) and has been modified extensively. Some of the modifications and/or extensions are RANDOM WALK (Prickett, Naymik, and Lonnquist 1981a,b), GWFL3D (Walton 1989), CONPLASM, and UNCPLASM.

The model and extensions reviewed in this report are those distributed by the IGWMC (IGWMC-FOS12). The model is distributed as a package of three finite difference codes: PLASM, CONPLASM, and UNCPLASM

and PREPLASM, a preprocessor. PLASM simulates two-dimensional transient flow of groundwater in heterogeneous, anisotropic, fully confined aquifers. CONPLASM is a modification of PLASM that solves two-dimensional transient flow in fully confined and leaky confined aquifers. UNCPLASM is a version of PLASM that solves the two-dimensional transient flow in unconfined or water table aquifers.

Overview. PLASM is a two-dimensional finite difference model that uses an iterative alternating direction implicit scheme in solving the governing unsteady-state groundwater flow in a confined, nonhomogeneous, and isotropic aquifer. The code is a block-centered model. PLASM requires the user to assign either storage coefficient or specific yield to the cell (area around the nodes) and to specify transmisivities to the cell faces (area between the nodes) (Anderson and Woessner 1992).

Evaluation. The code was evaluated with the four example data sets included with the documentation. One problem tests the no-flow boundary option, one the constant head option, a third tests the ability of running multiple wells, and the fourth is a regional groundwater system with multiple boundary condition options. The code was able to solve all four problems included in the documentation.

Hypothetical scenario. The model was tested with the WES Example 1 discussed in Chapter 3. Figure 20 shows the head distribution for the WES Example Problem 1. Overall, PLASM results compared favorable with results from other models like CSU-GWFLOW and RANDOM-WALK. Table 7 presents the difference between RANDOM-WALK and PLASM for confined and unconfined cases.

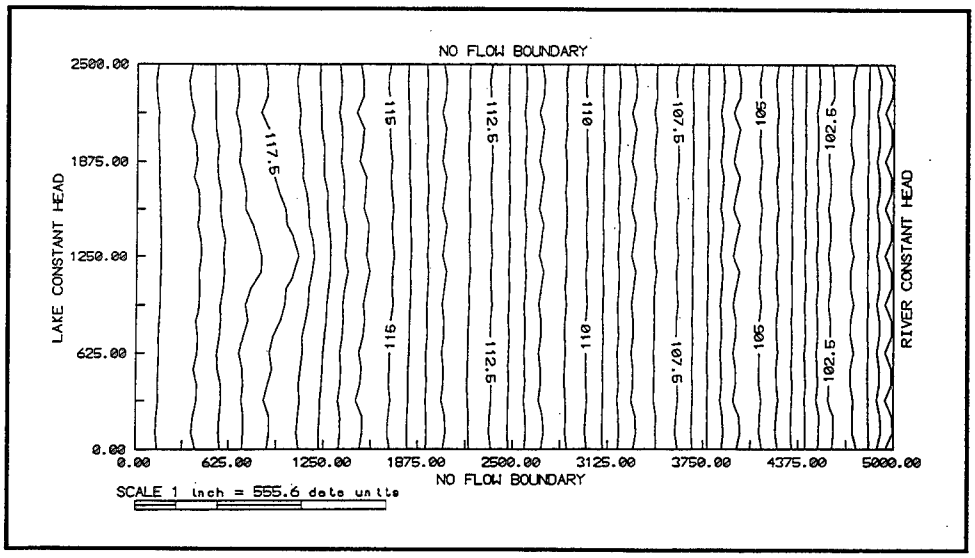

Figure 20. Head distribution for WES Example Problem 1

Table 7
PLASM and RANDOM-WALK Differences

Unconfined		Confined	
Recharge, Percent Difference	Pumping, Percent Difference	Recharge, Percent Difference	Pumping, Percent Difference
0.000	0.000	0.000	0.000
0.036	0.044	0.111	0.515
0.035	0.087	0.249	0.960
0.145	0.130	0.527	1.258
0.124	0.137	0.082	1.242
0.378	0.140	0.030	1.247
0.440	0.127	0.225	1.250
0.485	0.105	0.365	1.228
0.518	0.085	0.479	1.180
0.528	0.062	0.557	1.111
0.520	0.037	0.600	1.009
0.496	0.020	0.595	0.876
0.439	0.000	0.547	0.718
0.344	0.008	0.437	0.521
0.201	0.006	0.271	0.291
0.000	0.000	0.000	0.000

Summary. PLASM is a two-dimensional groundwater flow model. It is a mature code with significant support from third-party vendors. One third-party software used in the evaluation was PREPLASM, distributed by the IGWMC. PLASM is an excellent teaching tool and very useful in testing conceptual models. In an ideal world, a preliminary simulation would be performed with PLASM to adjust the major parameters, and then, after obtaining good agreement with site-specific data, a more comprehensive model would be run.

RANDOM WALK

The RANDOM-WALK algorithm for solving solute transport in groundwater was developed by Thomas Prickett of the Illinois State Water Survey (Prickett, Naymik, and Lonnquist 1981a,b). The original RANDOM WALK model consisted of PLASM coupled with a "random walk" solute transport model. The model simulates one- or two-dimensional contaminant transport. The transport of contaminants is simulated by moving "particles" with both advection and dispersion. It uses groundwater velocities to compute the advection part of the displacement and a MONTE CARLO method for

determination of displacement due to dispersion. In addition, the model simulates the effects of chemical reactions.

The RANDOM-WALK algorithm has been coded into both two-dimensional (RAND2D)[1] and three-dimensional (RAND3D) models. Comparisons of the two-dimensional (RANDOM WALK) model with analytic solutions for three cases was performed by Beljin (1988). Beljin (1988) used the IGWMC version of RANDOM WALK (original model). RAND3D and RAND2D are modifications of the original RANDOM WALK by Thomas Prickett and other contractors.

Objective. The first objective of this study was to test both the IGWMC version of RANDOM WALK and the three-dimensional solute transport model RAND3D using three test cases:

a. A continuous source in a constant flow field (Case 1).

b. A slug source in a constant flow field (Case 2).

c. A continuous source in a constant flow field (Case 3).

These cases correspond to three cases used in Beljin (Beljin problems BM-I.3 (fine grid), BM-I.4, and BM-I.5 correspond to Case 1, Case 2, and, Case 3, respectively). In order to compare RAND3D with the two-dimensional results, the three-dimensional model aquifer was set up to be, in essence, a two-dimensional problem. This meant that there was no variation in geohydrologic parameters in the x-y plane.

The second objective was to determine the degree of difficulty in using RAND3D and its applicability to complex groundwater geometries. To avoid duplication of efforts, the IGWMC version of RANDOM WALK was only tested against the sample data sets included with the distribution diskette.

Overview. RANDOM WALK was evaluated to level one following the protocol described in Chapter 2. The manuals included in the IGWMC version were Bulletins 55 and 65 from the Illinois State Water Survey (Prickett and Lonnquist 1971; Prickett, Naymik, and Lonnquist 1981a,b). The documentation was good. The model is an adaptation of the mainframe code RANDOM WALK developed by Prickett, Naymik, and Lonnquist 1981a,b. The code is written in FORTRAN and was compiled with Microsoft FORTRAN Version 3.2.

The model was tested against the three examples included in the distribution diskette. The results were satisfactory when compared against the results in the original manual. RAND3D was selected for further evaluation (level two) because the model is an extension into three dimension of the original one- or two-dimensional RANDOM WALK.

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[1] Prickett refers to the two-dimensional model as TRANS. For consistency with RAND3D, TRANS will be referred to as RAND2D.

There are significant limitations to the use of RAND3D as it exists at present. These limitations concern the type of platform the code must run on and the maximum size of the problem allowed.

RAND3D is written in BASIC and must be run on IBM-PC or compatible machines under the MS-DOS operating system. The machine must have 640 K of memory. It is an interactive program that uses the Microsoft Quick BASIC graphic routines. This limits the use of the program to fairly small, simple problems. Larger, more complicated problems would require more layers, more grid points, and more particles. The present limits are 3 layers, 40 rows, 40 columns, and 10,000 particles. In addition, larger problems in the foreseeable future will require significant amounts of computer time. It would be preferable to run these on mainframes or work-stations. In order for this to be done, the code must be rewritten so that it is completely portable. This would require conversion to a standard language (FORTRAN or C) and the removal of machine-dependent graphics.

Input/output parameters. RAND3D requires that at least two layers be defined. In order to make comparisons with the two-dimensional cases, transport should only be in a single, homogeneous aquifer. This was simulated by defining the lowest layer (layer 1) in RAND3D such that no transport occurred there. This was accomplished by setting the sources exclusively in the second layer, defining the vertical dispersion in all layers to be 0, and setting the flow velocities in the lowest layer to 0. Also, the vertical velocities in all layers were set to 0.

Case 1, Continuous Source in a Constant Flow Field:

This case used an aquifer with the following geohydrologic and model parameters:

aquifer thickness, b	110 ft (undefined in 2-D case)
Darcy Velocity, v	0.525 ft/day
Porosity, n	0.35
Mass/Particle, M	29.12 lb/particle
Particles	5,000
Time	2,800 days
Total Mass Injected	52 lb
Dmax	10 ft
Zmax	1 ft
Longitudinal Dispersivity, α_L	70 ft
Transverse Dispersivity, α_T	14 ft
No Retardation	
No Decay	
Number of Rows (Y dimension)	19
Row Spacing	98.4 ft
Number of Columns (X dimension)	36
Column Spacing	196.8 ft

The source of contamination is a continuous source along a line that is centered at X = 500 ft, Y = 900 ft and is throughout the second aquifer layer (110 ft).

Figure 21 shows the RAND3D, RAND2D, and the analytic solutions of Case 1 for a cross section through Y = 900 ft. This shows good agreement with both the two-dimensional and analytic solutions. Figure 22 shows

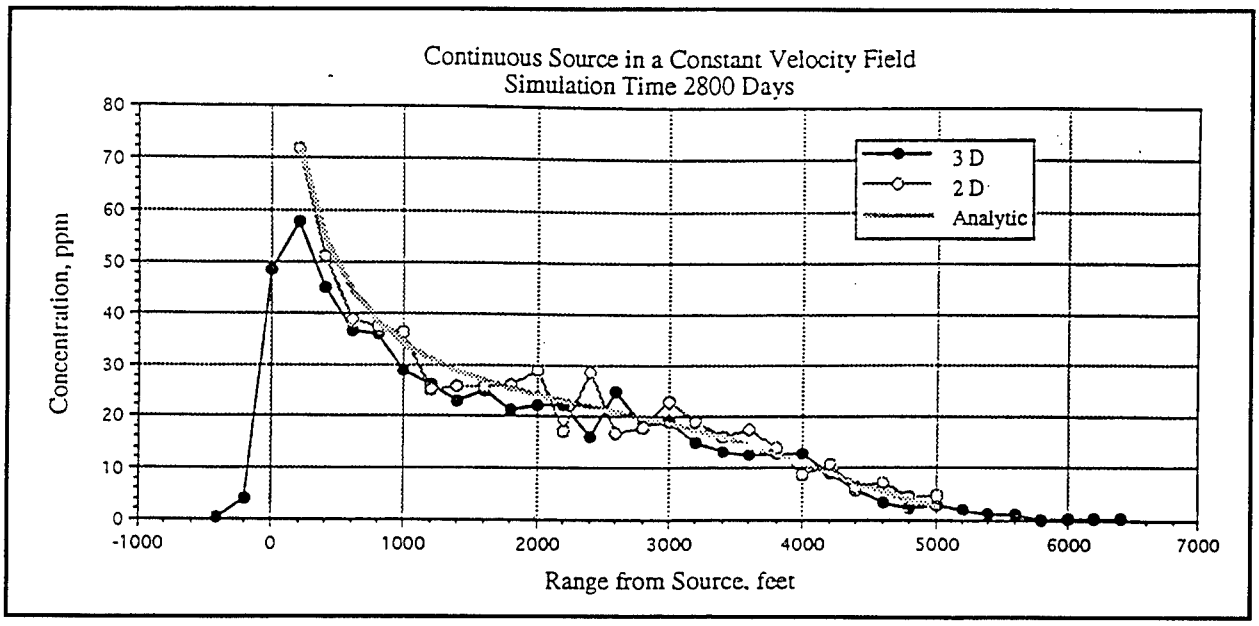

Figure 21. Simulation of a continuous source, Case 1 at time 2,800 days

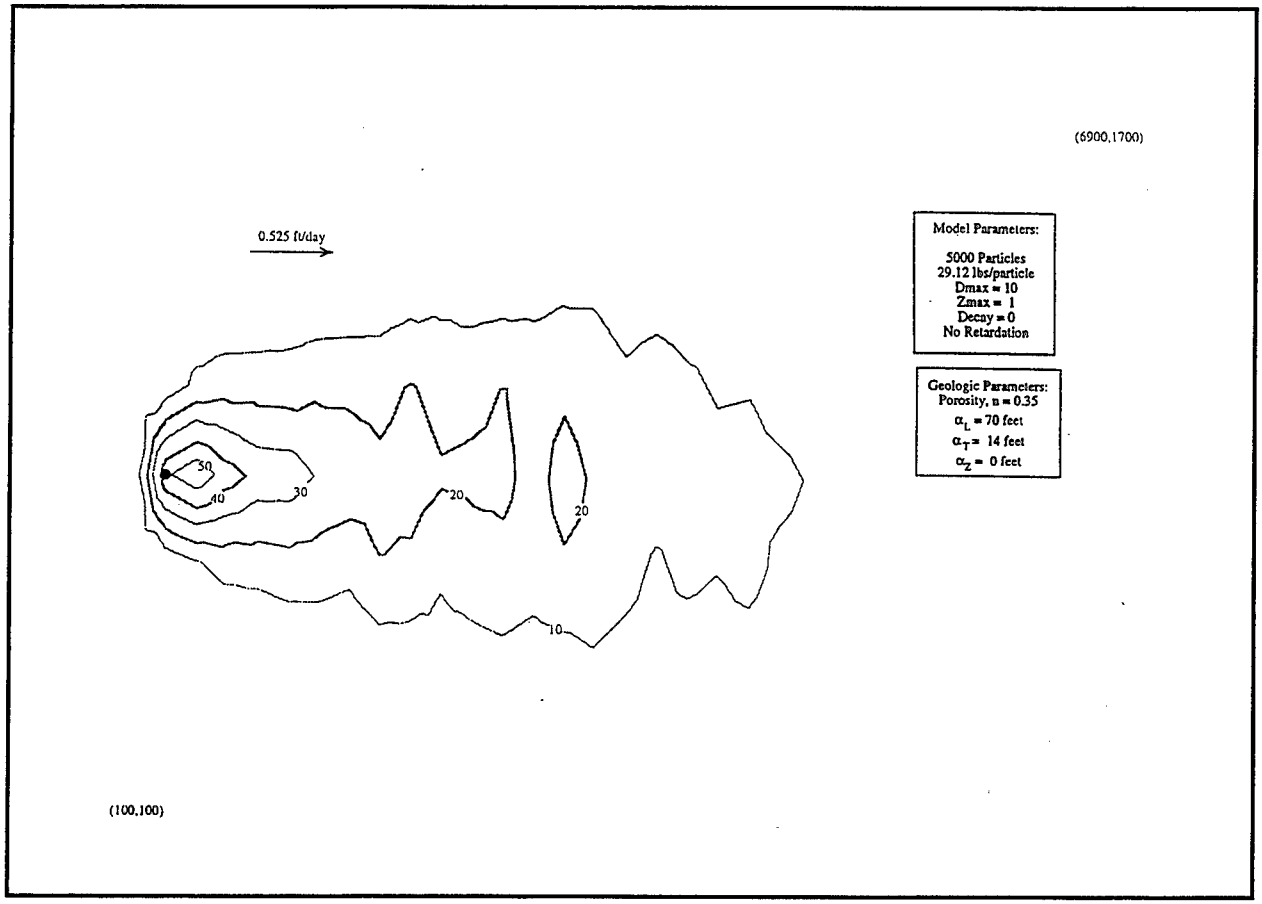

Figure 22. Concentration contours, Case 1 at time 2,800 days

the RAND3D-predicted plume formed by the source at a simulation time of 2,800 days. Note that it is not symmetric. This is due to the random nature of the solution technique. This random nature of the model also explains why there is mass upstream from the source. One of the characteristics of the RANDOM-WALK method is that one will get a slightly different answer every time it is run. Figures 23 and 24 illustrate this point. These simulations were done using the same identical inputs (note that the parameters are not identical with the parameters above), but were done at different times. There are variations. There are two possible solutions to this problem. The first is to increase the number of particles used. The second is to do multiple runs and compute the average (and perhaps standard deviation).

Case 2, Slug Source in a Constant Flow Field:

This case used an aquifer with the following geohydrologic and model parameters:

aquifer thickness, *b*	32.81 ft
Darcy Velocity, *v*	6.56 ft/day
Porosity, *n*	0.35
Solute Mass/Unit Thickness	2.35 lb/ft
Total Mass Injected	77.1 lb
Mass/Particle, *M*	0.03281 lb/particle
Particles	2,350
Times	3.96 days
	10.59 days
	16.59 days
Dmax	3 ft
Zmax	0.3 ft
Longitudinal Dispersivity, α_L	13.12 ft
Transverse Dispersivity, α_T	3.28 ft
No Retardation	
No Decay	
Number of Rows (Y dimension)	19
Row Spacing	16.4 ft
Number of Columns (X dimension)	40
Column Spacing	16.4 ft

The source of contamination is a slug source along a vertical line that is located at X = 57.4 ft, Y = 156 ft and is throughout the second aquifer layer (32.81 ft).

Figures 25, 26, and 27 show the RAND3D, RAND2D, and the analytic solutions for this case at three different times: 3.96, 10.59, and 16.59 days. The three-dimensional solution agrees well with the analytic solution as well as the two-dimensional solution. There appears to be slightly more deviation from the analytical solution at the early times (3.96 days) than for the 10.59 and 16.59 days. For short time periods, the discreteness of the model will be more evident; therefore, the results will deviate more. However, as the simulation time increases, the discrete particles will be smoother, and there will be less variation.

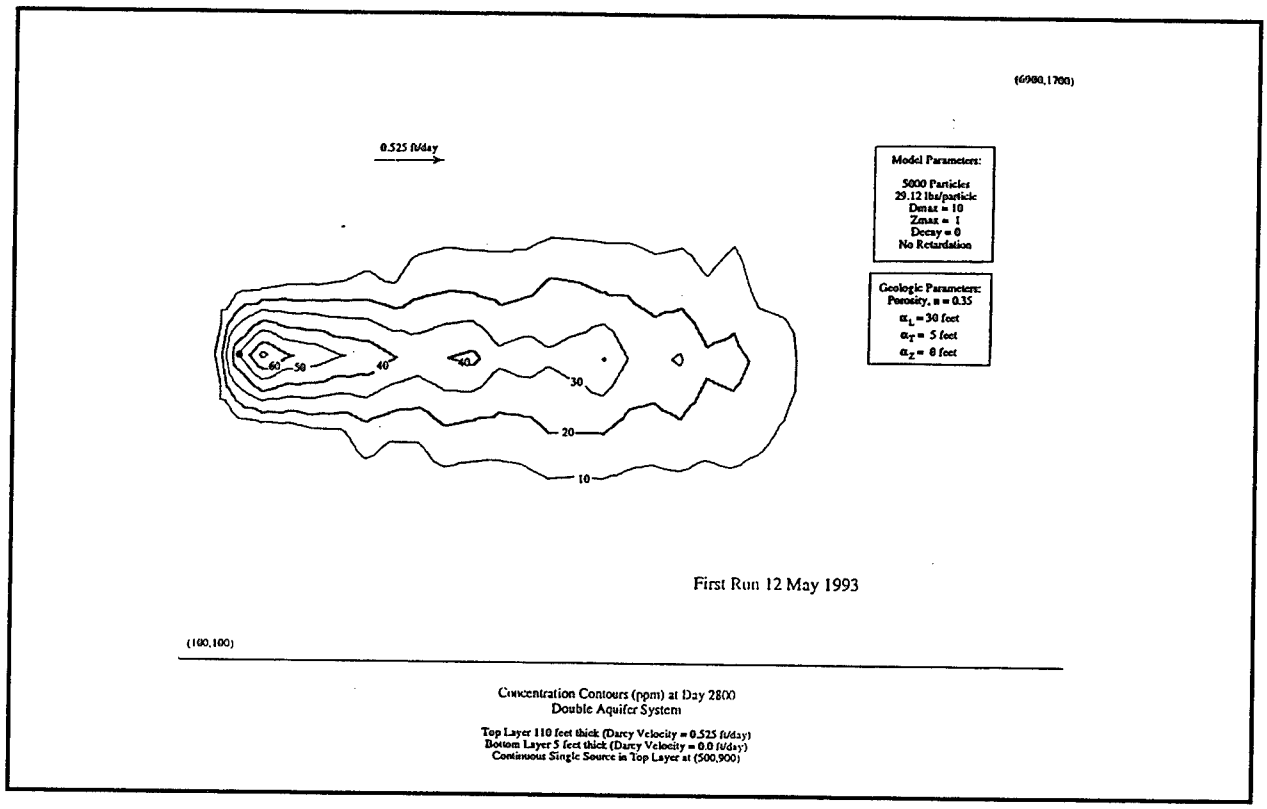

Figure 23. Comparison of solution technique, Run 1 concentration contours

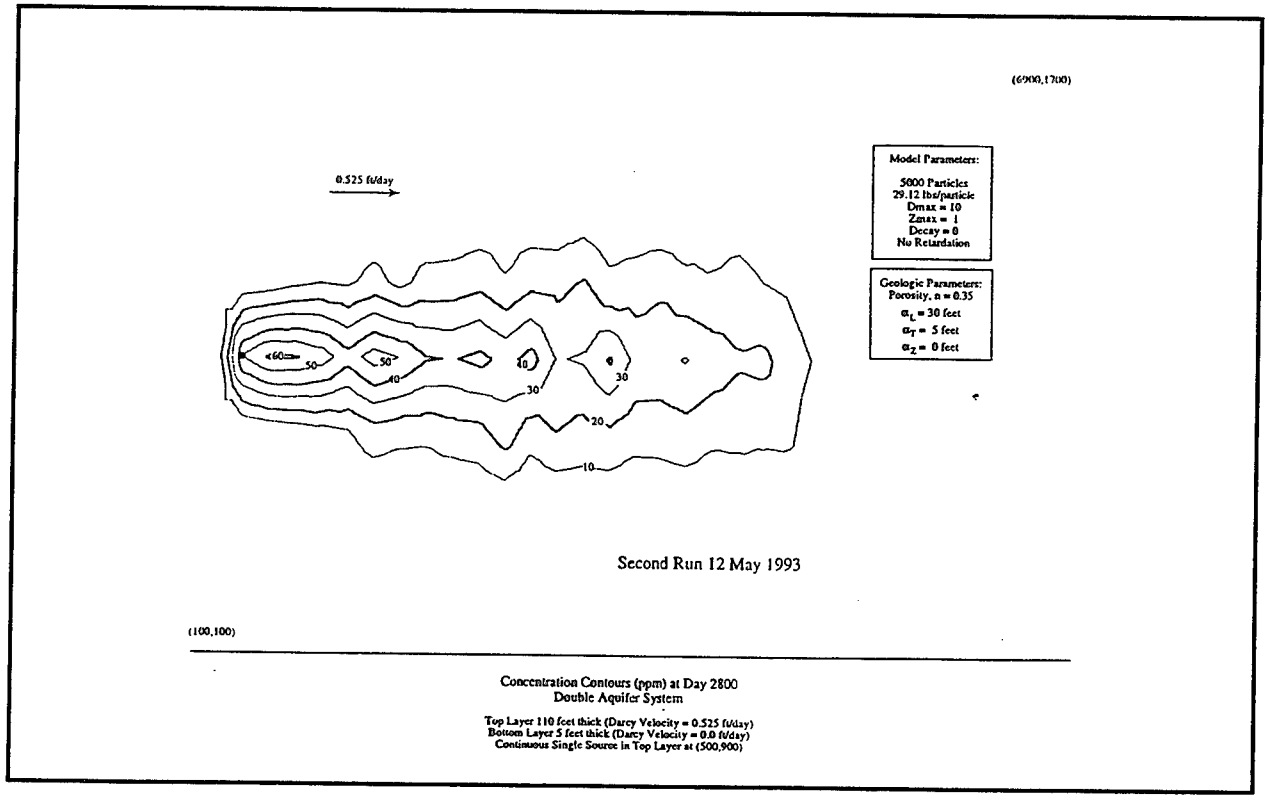

Figure 24. Comparison of solution technique, Run 2 concentration contours

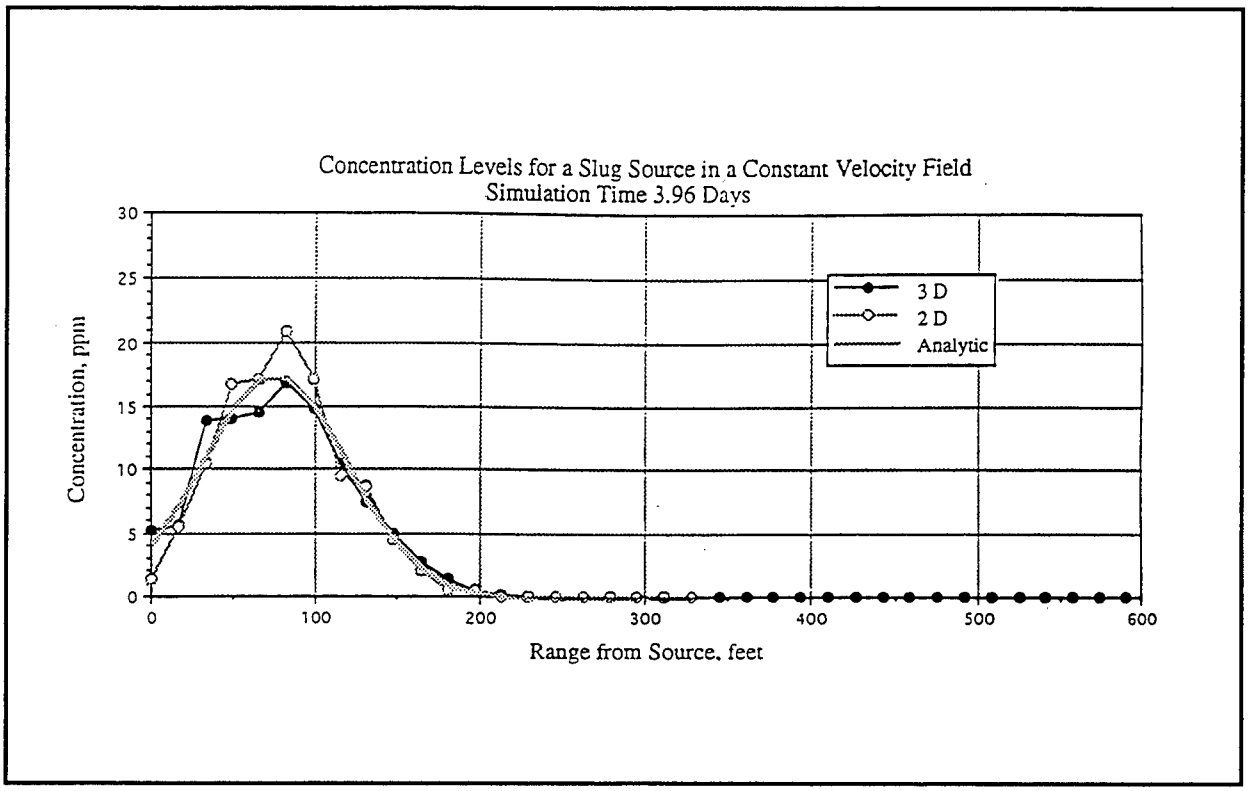

Figure 25. Simulation of a slug source, Case 2 at time 3.96 days

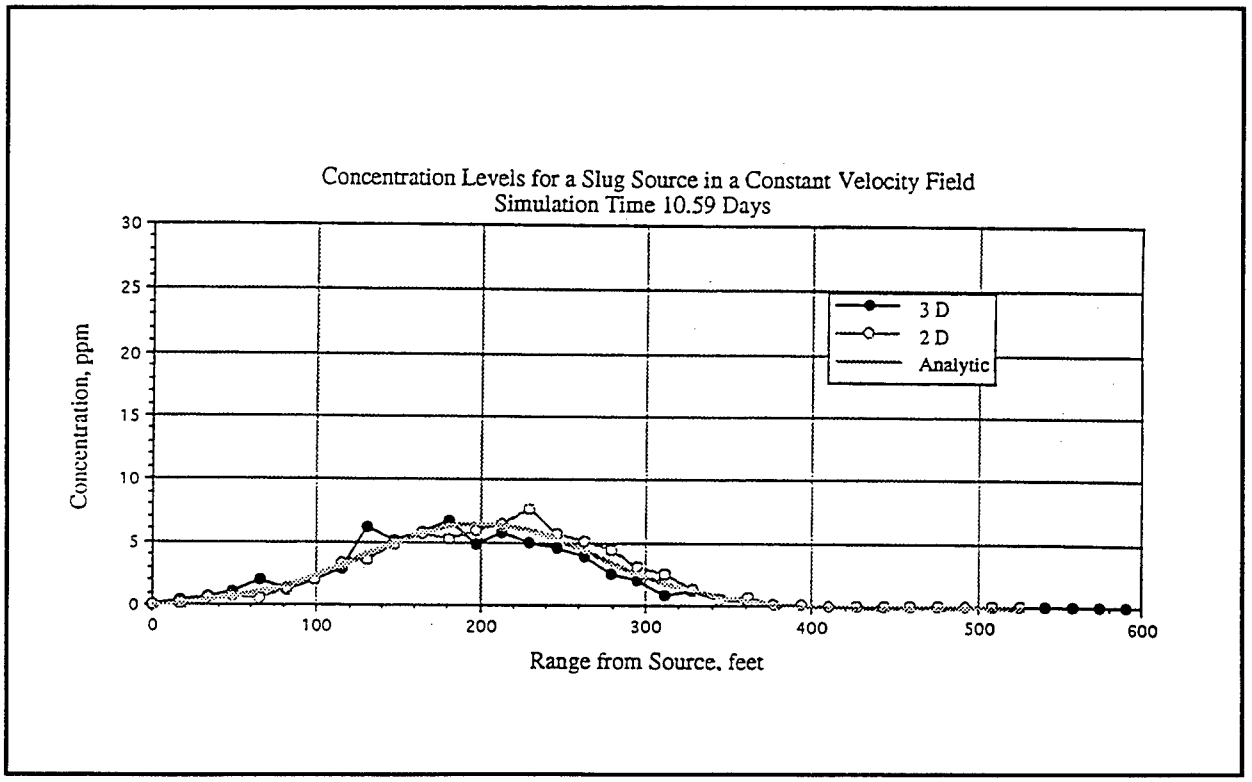

Figure 26. Simulation of a slug source, Case 2 at time 10.59 days

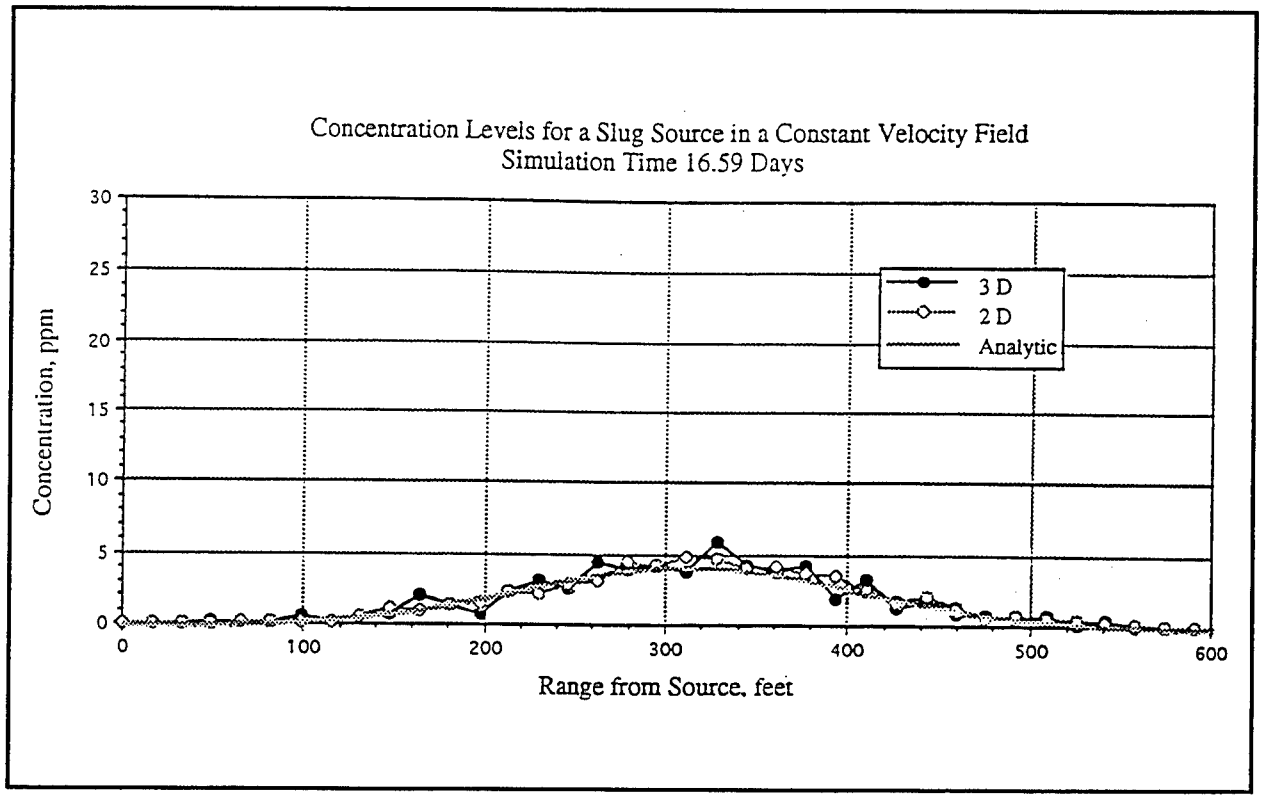

Figure 27. Simulation of a slug source, Case 2 at time 16.59 days

Case 3, Continuous Source in a Radial Flow Field:

This case used an aquifer with the following geohydrologic and model parameters:

aquifer thickness, *b*	32.81 ft
Inflow, *Q*	882.83 ft^3/day
	6,610 gal/day
Porosity, *n*	0.25
Total Mass Injected	200 lb
Mass/Particle, *M*	0.8 lb/particle
Particles	10,000
Times	20 days
	40 days
Dmax	0.6 ft
Zmax	0.06 ft
Longitudinal Dispersivity, α_L	0.984, 0.492, 0.049 ft
Transverse Dispersivity, α_T	0.246, 0.123, 0.012 ft
No Retardation	
No Decay	
Number of Rows (Y dimension)	39
Row Spacing	3.28 ft
Number of Columns (X dimension)	39
Column Spacing	3.28 ft

This case provided a problem not encountered in the previous cases. The velocities in the computational grid were determined by the inflow rate (Q) and the distance from the well. The formula used for the velocity magnitude was:

$$V = Q/A \tag{27}$$

where

Q = inflow, 882.83 ft^3/day

A = area of a cylinder defined by $A = 2\pi Rb$
R = distance from well
b = aquifer thickness, 32.81 ft

The solution is acceptable for all the locations except at the well itself. Since the velocity magnitude is inversely proportional to R, as $R \rightarrow 0$, $V \rightarrow \infty$. Therefore, velocities near the injection well will be interpolated using extremely high values. To avoid this, one can either set the velocity at the well to 0 or set the radius at a distance so that all particles start with reasonable velocity values. If the velocity at the source were set to 0, then the program crashes. This is because the dispersion term depends on the velocity. This meant that the source could not be a line (as in the previous two cases). The only way to run this case was with the source defined as a cylinder with its center at X = 63.96, Y = 63.96, and a cylinder height equal to 32.81 ft. Figure 28 illustrates the location and size of the cylinder and also the velocity magnitudes. The radius of the cylinder (well radius) had to exceed 4.64 ft in order to avoid the velocity interpolation routines use of the velocity at the well.

The method in which RAND3D distributes the particles around the cylinder is supposed to be in a uniform pattern. The results, shown in Figures 29-34, indicate that there might be a problem in the routine that determines the particles starting point. The solution is not symmetric. These results cannot be accounted for even if the assumption is made that there will be a certain lack of symmetry due to the random nature of the solution. The problem could be with the routine that determines the particle starting points or with the random number generator of the computer.

It should be noted that in the original test case for the two-dimensional model, the transverse dispersivity, α_T, was set to 0. When RAND3D is run with this value, every particle travels in a straight line away from the source. It was decided to use a value of $\alpha_T = \alpha_L/4$ in order to get results that made sense. However, even with the highest values of α_T and α_L, the asymmetry exists in the results. Comparison with the two-dimensional and analytic results would be meaningless, as they would depend on values along an undefined line through the center that could be chosen to give any degree of agreement.

Summary. Once a user becomes familiar with RAND3D, it is fairly easy to run. It is also fairly easy to enter erroneous input parameters, like any other codes, and in some cases, one must let the program finish a simulation; it can be corrected.

When particles reach the model boundary, they "bounce" back. Extending the boundaries helps in avoiding the "bounce" back; this requires either increasing the row or column spacing or the number of rows or columns. Such modifications can affect the resolution and/or execution time.

The user may even need to recompile with larger dimensions in the arrays, in which case he would need to have Microsoft Quick BASIC compiler.

The code is limited to use on IBM-PCs or compatibles. This limits the size to 640 K. For large complex problems requiring long simulation times and many particles, using PCs may also be inconvenient. A lot of the limitations are probably addressed in the code's recent release.

Multiple time simulations of continuous sources runs require that the simulations start at time 0. You must also reinitialize the particles, or they will start where they were at the end of the last time simulation (re-setting the time to 0 does not reset the particles to their original locations).

Truly complex problems, with many layers with different geohydrologic parameters are not easy to run with RAND3D. It allows only single porosity and dispersivity values throughout the domain. In addition, if there are cells with no velocity, particles that enter will never leave that cell.

Saving data requires you to define a constant x-y increment and number of rows. This requirement is not very useful since a grid has already been defined. In fact, if your computational grid has a $\Delta x \neq \Delta y$, you must define an increment that is at least as large as the largest of the grid increments. This means that you smooth some of the results.

Modeling large remediation projects with this model would be very time-consuming for the untrained user. Modifications to take care of some concerns mentioned above would make RAND3D more useful. A new version of RAND3D was recently released that may address some of the weaknesses.

Unsaturated Flow and/or Transport Models

UNSAT1

The model UNSAT1 is a one-dimensional finite element model for variably saturated soil profiles. It is distributed by the International Ground Water Modeling Center (IGWMC) located in Golden, CO. The current model being distributed is Version 1.0 and was written by M. Th. van Genuchten. The IGWMC charges a nominal fee for the software to cover the costs of distributing the program and documentation. The UNSAT1 model can be obtained by writing to the following:

IGWMC
Institute for Ground-Water Research & Education
Golden, Colorado 80401-1887, USA
Phone: (303) 273-3103

The UNSAT1 model is a generalized Hermitian finite element computer model. It can be used to simulate variably saturated moisture movement in one dimension. Furthermore, the model can be applied to both

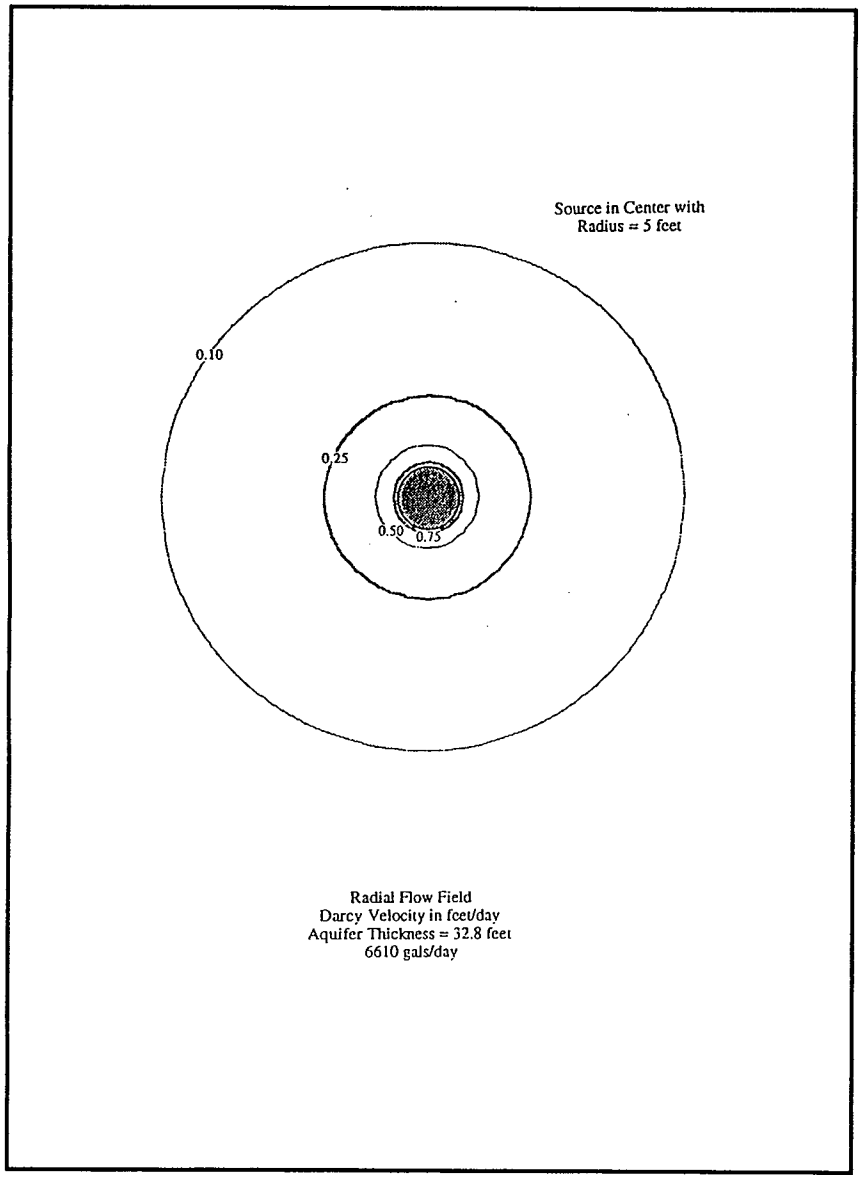

Figure 28. Continuous source in a radial flow field, Case 3

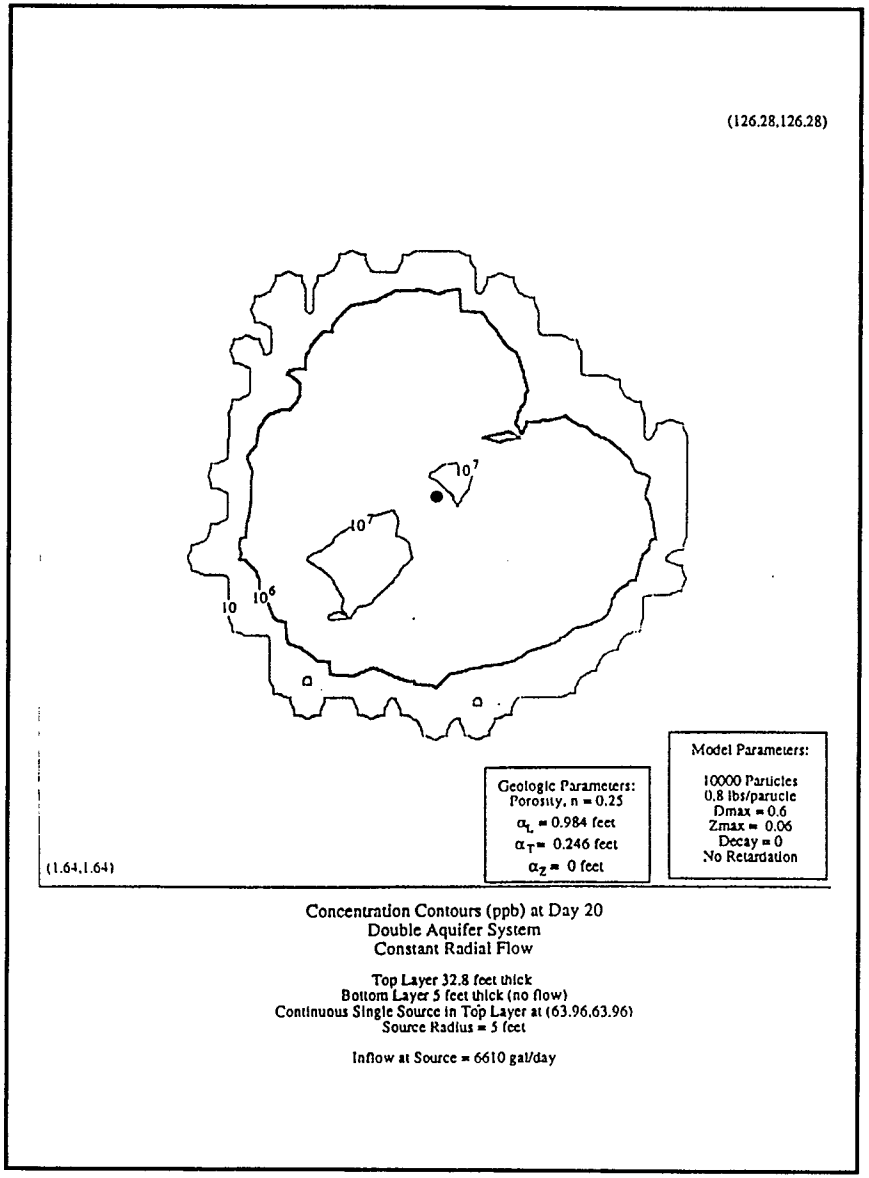

Figure 29. Concentration contours, Case 3, Test 1 at Day 20

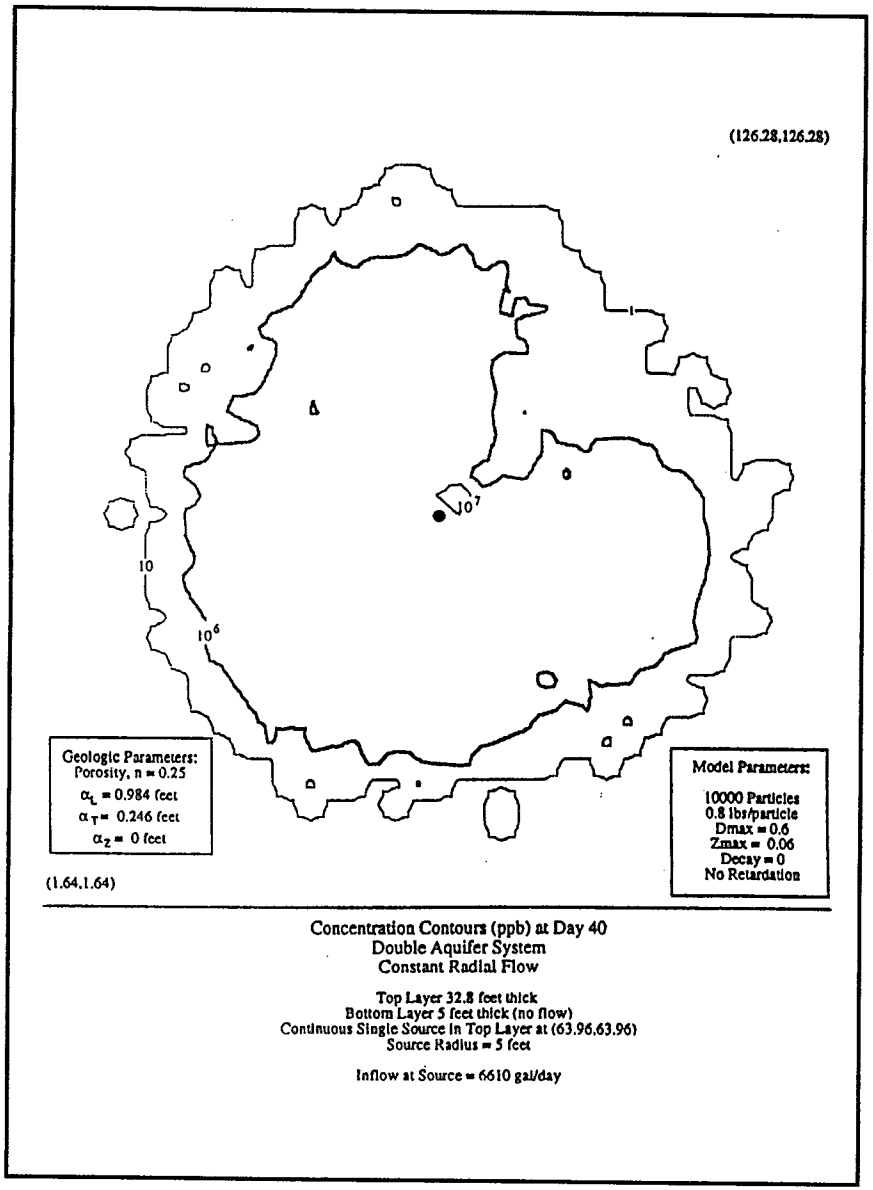

Figure 30. Concentration contours, Case 3, Test 1 at Day 40

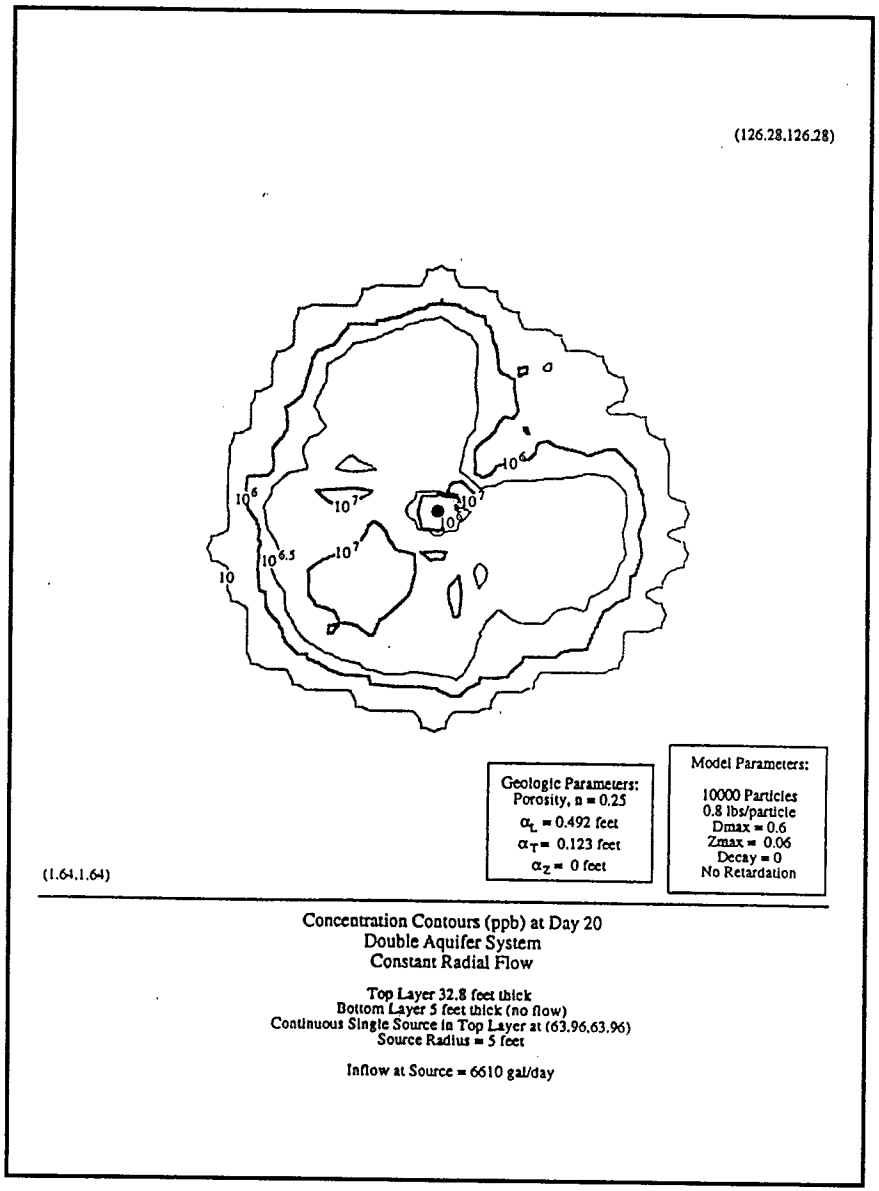

Figure 31. Concentration contours, Case 3, Test 2 at Day 20

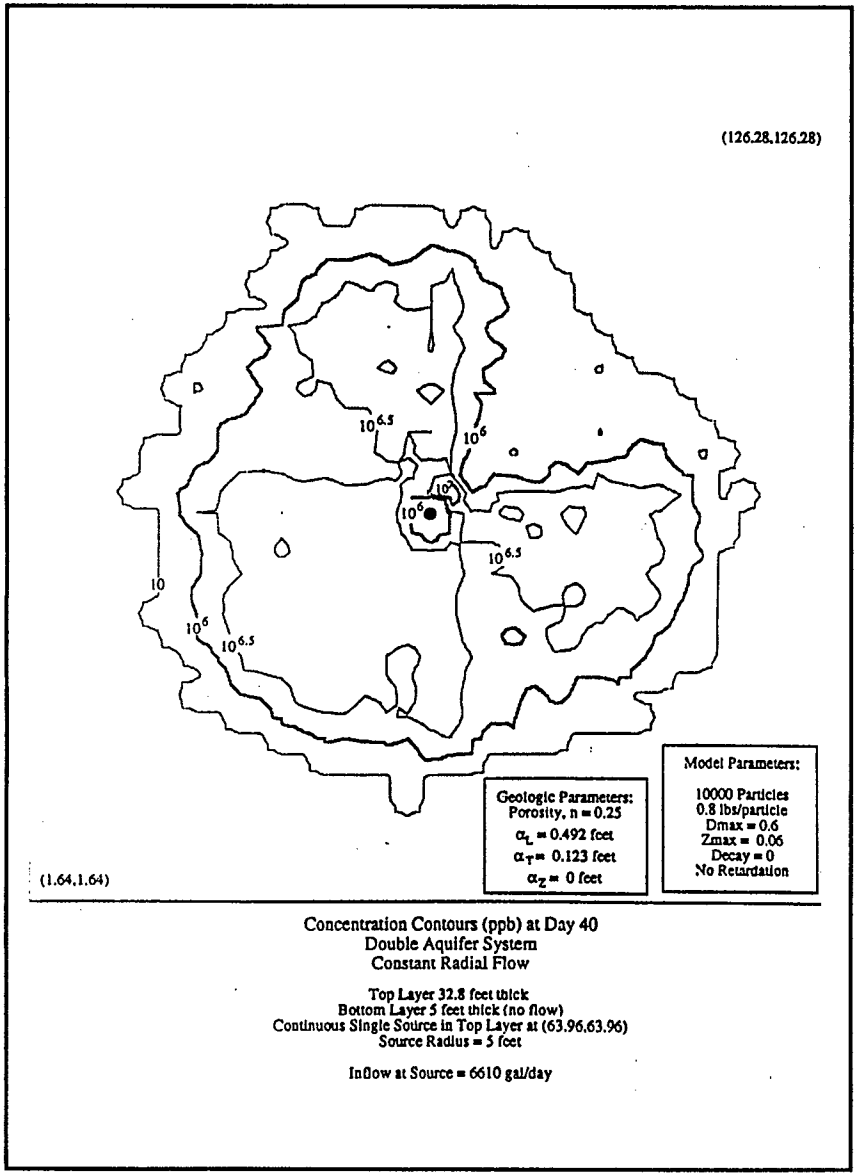

Figure 32. Concentration contours, Case 3, Test 2 at Day 40

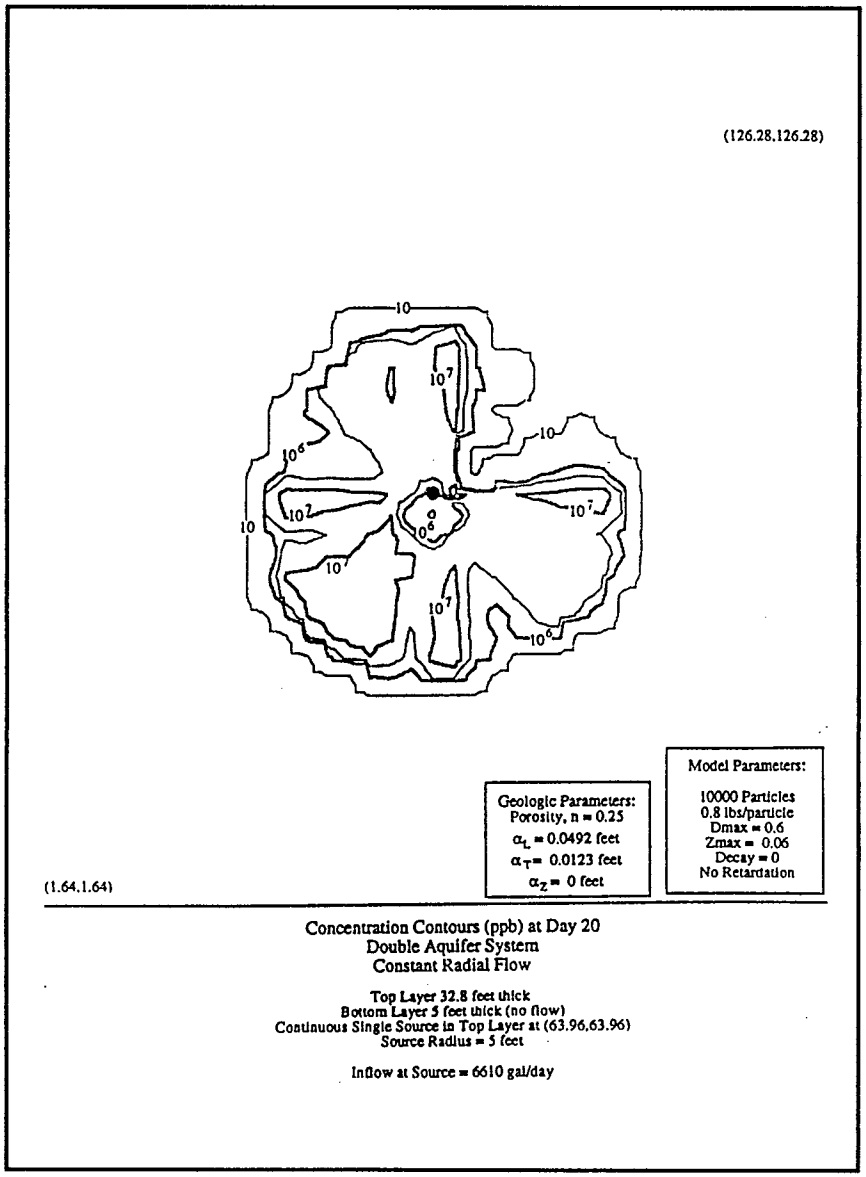

Figure 33. Concentration contours, Case 3, Test 3 at Day 20

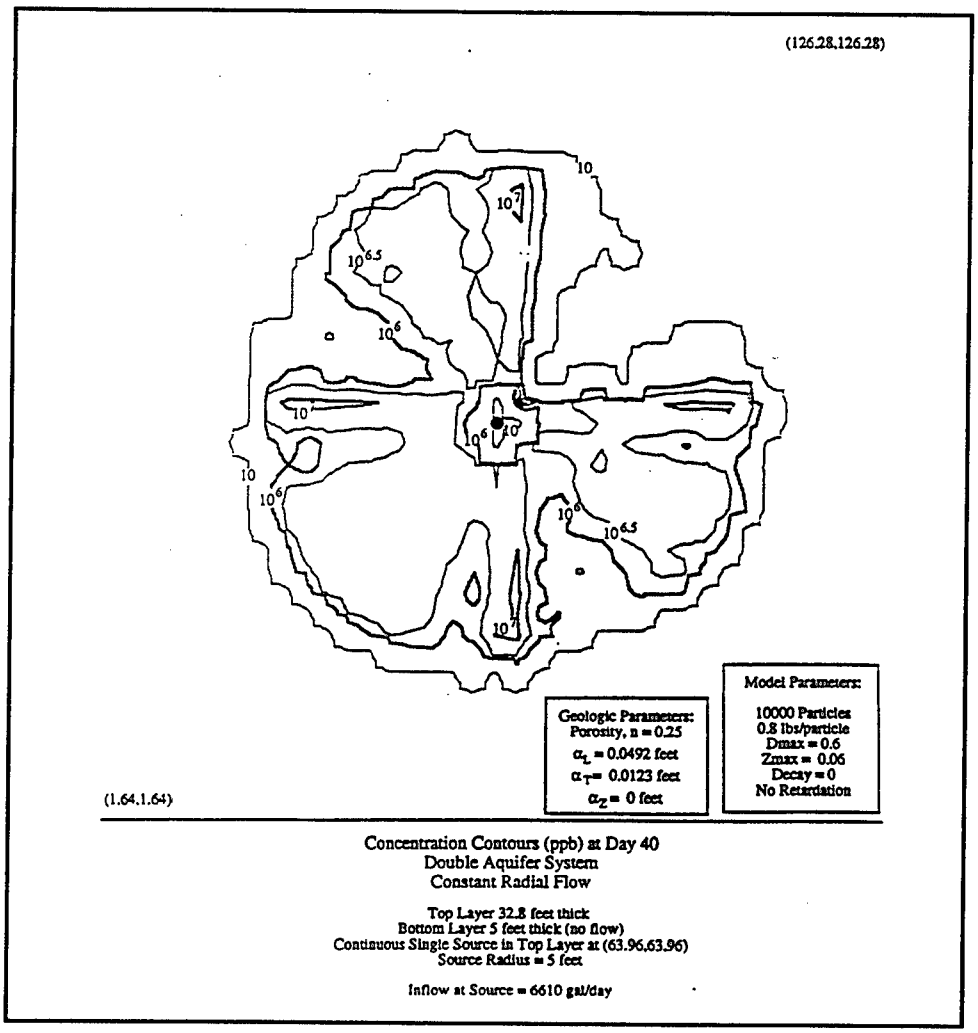

Figure 34. Concentration contours, Case 3, Test 3 at Day 40

homogeneous and nonhomogeneous soil profiles, enabling the user to analyze moisture movement in soil profiles containing abrupt and smooth changing profiles. The UNSAT1 model was written in FORTRAN, and the currently executable file being distributed was compiled using Microsoft FORTRAN Version 3.2. The operation of UNSAT1 has the following run time requirements:

- IBM-PC, XT, or AT
- 512K RAM
- DOS 2.0 or higher
- Intel 8087 or 80287 Numerical Coprocessor
- One floppy disk drive

The model, as currently distributed by the IGWMC, includes both executable and source code files. The source code is supplied to permit users to alter the program to meet specific programming needs not handled in the distributed version of UNSAT1 and for modification of the BC

(boundary conditions) subroutine and SPR (soil property) function. The BC subroutine and SPR function are problem dependent and must be modified for user-defined data sets. The BC subroutine defines the transient boundary condition at the soil surface, and the SPR function calculates soil hydraulic properties. In general, most UNSAT1 applications require input data set creation and BC and SPR modification. Modifying the UNSAT1 program will require the use of a FORTRAN compiler, which is not provided by IGWMC. Other files that are supplied include an input and output data set and a postprocessor program. The postprocessor program can be used to remove carriage controls from the output data set. In addition, a software product description detailing model application is included. Notices describing changes in the original source code of UNSAT1 are provided by IGWMC, which maintains a list of licensed users.

Overview. The computer model UNSAT1 was written to allow for simulation of moisture movement in a one-dimensional variably saturated soil profile. The soil profile can be nonhomogeneous, permitting a variety of soil properties. Currently the model only simulates moisture movement and not chemical transport.

Files distributed from the IGWMC include UNSAT1.FOR, UNSAT1.EXE, UNSAT1.DAT, UNSAT1.OUT, STRIP.FOR, STRIP.EXE, and UNSAT1.DOC. The FORTRAN source code for UNSAT1 is listed in the UNSAT1.FOR file. The compiled version of this code is the UNSAT1.EXE file. It was compiled using Version 3.2 of Microsoft FORTRAN. The program can be tested by running the example data set UNSAT1.DAT and then comparing the generated output data set to the file UNSAT1.OUT. The two output files should be identical. Carriage controls can be removed from the output data set by using the STRIP.EXE program. The STRIP.FOR is the source code for the executable file, and cleans up the output data set by executing the carriage control commands. Finally, UNSAT1.DOC contains the information required to run the program as well as a description of the software product.

The UNSAT1 program was developed using a Galerkin finite element technique to solve the variably saturated flow equation. A series of basis or shape functions were used to approximate the dependent variables, pressure head or moisture content. First-order continuous cubic (Hermitian) polynomials were used as the basic functions for the one-dimensional, variably saturated flow equation.

Input/output parameters. Operation of the UNSAT1 model requires a single input data set and the executable file UNSAT1.EXE. Upon typing the command UNSAT1, the user will be prompted for the names of the output file name (unit 6) and input file name (unit 5). The supplied input file, UNSAT1.DAT, should be used for the first run to ensure that the model is operating correctly. Any output file name can be used. After the run, the output file created should be compared with the UNSAT1.OUT file to verify the run. The output files should be identical.

The compiled version of UNSAT1.EXE is for example problem 2 in the user manual. The moisture model used for this problem and the UNSAT1 program is based on equations developed by van Genuchten (1978). The equations require information pertaining to soil hydraulic properties. The

distributed version of UNSAT1.EXE uses soil hydraulic properties for the soil layers of problem 2. Again, for user-specified problems, the subroutine BC and function SPR must be modified. These files contain information relating to boundary conditions and soil hydraulic properties. After alteration, a new UNSAT1.EXE file needs to be created by compiling the user-modified version of the UNSAT1.FOR file.

The input data set for the UNSAT1 model follows the FORTRAN 77 format statements. Table A2 in the users manual provides the information regarding the format structure for each column entry. Descriptions of the variables contained in the file are further described in Table A1. Information contained in the input file includes global parameters, time steps, boundary and initial conditions, and soil properties. New input files can be created be modifying the distributed input data set or by creating a new one following the structure outlined in Table A2.

The output data are written to the file specified by the user as "unit 6" when running the program. The output file contains descriptions of the input parameters, surface moisture values, initial conditions, and soil hydraulic properties. Following this information, the pressure head and moisture contents are given for each depth (node) at each time interval specified by the user in the input data set. This information can then be used to graph pressure distributions produced during the simulation. The output data set produced when running UNSAT1 is given in Table A4 in the manual. Following the computer run, the user can then use the STRIP.EXE postprocessor program. This program removes or executes the FORTRAN carriage controls from the UNSAT1.OUT or output file. The program will prompt the user for the file created upon running the UNSAT1.EXE program, and a new name must be assigned to the file created using the strip program. The STRIP.EXE program will overwrite the original input data set if that file name is used. The output from the simulation can be sent directly to a printer by specifying unit 6 as the local printer (lpt1).

Evaluation. The author reported run times of approximately 25 min. However, the type of machine it was run on was not mentioned; thus, direct comparisons cannot be made. The time for a run will vary based on factors such as number of soil layers, time intervals, and the computer used. For example, running the same example data set on a Gateway 2000 4DX2-66V microcomputer (486-66 MHz) took only 25 sec as compared with the 25 min reported in the documentation.

Summary. The example data set supplied with the model ran without difficulty. The output file created running the program matched the output file provided with the documentation indicating a successful simulation. Moisture content profiles created using output from the simulation produced graphs that were reasonable and within physical expectations for a moisture model.

The input data sets for the UNSAT1 model are rather difficult to set up; thus, the model could be greatly enhanced with a preprocessor to aid in the creation of input files. Currently, the input data sets are either created from scratch or by editing an existing input file. The tendency for mistakes creating these files is great. Any extra character outside of the format

field will create errors terminating the program. The program does not give clues regarding the location of the error in the input data set, and much time can be lost searching for mistakes. A preprocessor could create these input files, reducing the time and effort required in the structuring of input data sets.

The UNSAT1 model can be used to simulate moisture movement in a one-dimensional, saturated-unsaturated, homogeneous-nonhomogeneous soil profile. The model does not handle contaminant transport. However, the output from the model can be used to provide moisture profiles, which could then be used as input for a contaminant transport model.

CHEMFLO

CHEMFLO is a software system designed to define, solve, and display the water and chemical movement in the unsaturated or vadose zone. The system was developed for the Robert S. Kerr Environmental Research Laboratory (Nofziger et al. 1989). The software system is intended as both a teaching tool and a decision-making tool.

The software system was developed for the PC environment. The model requires 640K of RAM to run and needs the ansi.sys device driver loaded in order for the screens to be legible. The software system was evaluated on a 486/66MHz IBM PC compatible computer. The software/ hardware requirements to run the software system are as follows:

- IBM PC, AT, PS2, 386 or 486 compatible microcomputer.
- MS-DOS or PC-DOS Version 2.01 or higher.
- 640K base memory.
- Two floppy disk drives or one floppy disk drive and one fixed disk.
- An 80X87 math coprocessor is highly recommended.

The software system consists of a pair of partial differential equations to solve for water and chemical movement. The water flow is described using Richard's equation to solve the one-dimensional water movement in unsaturated soils. Chemical movement, sorption, and degradation are described by solving the convection dispersion equation. The two equations are solved numerically using finite difference.

The major model assumptions include homogeneous soil properties, instantaneous and reversible chemical partitioning, first-order degradation rate in both the liquid and solid phases, zero-order degradation rate constant for the liquid phase, and negligible hysteresis in the wetting and drying processes. The model can simulate both drainage and desiccation of a soil. Four soils are included in the soil database, a part of the software system. The soil database can be easily modified to include other soils and their properties.

Input/output parameters. The model requires input parameters defining the soil conditions, the chemical properties and characteristics, and the water system. Boundary conditions for water flow may be defined at

the upper and lower soil surfaces. Three types of boundary conditions can be applied at the soil surfaces. At the upper and lower surfaces, the boundary conditions can be specified as constant potential, constant flux, and mixed type. In addition, a fourth boundary condition, called the rainfall boundary condition, can be applied at the upper soil surface.

The program allows the user to select one of several moisture-retention models like Brooks-Corey, van Genuchten, Haverkamp, and Brutsaert. Analogous models are available to describe the hydraulic conductivity-moisture content relationships. The user must provide the coefficients used to fit the moisture retention models. The four soils included in the soil database have "typical" coefficients that could help the user in selecting appropriate coefficients. However, the coefficients used in these moisture-retention models should be fitted from field data if available, since the coefficients range is significant.

Two types of boundary conditions for chemical simulation can be specified at the soil surface. Constant chemical concentration in the inflowing solution may be specified. A constant concentration at the soil surface may be specified. That is, the concentration at the upper surface is held constant over time. Initial chemical concentration in the soil column may vary with depth.

Output from CHEMFLO may be in both graphical and tabular form. Graphical displays include matric potential, conductivity, saturation, flux density, and driving force with depth and/or time. The user can select from a variety of graphs for screen displays and tabular output. Runs can be saved into "simulation" files; the tabular output, if selected, then takes the same name with the TAB ending (i.e., "filename.TAB"). The size of the tabular output can be significant. Attention to both the time step and the tabular output time step is needed.

Equations. The partial differential equation used to describe one-dimensional water movement is that of Richards (Nofziger et al. 1989):

$$\frac{d\theta}{dh}\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} - \cos(A)\right)\right] \tag{28}$$

where

$h = h(z,t)$ = matric potential

z = distance coordinate parallel to flow direction

t = time

$\cos(A)$ = cosine of angle between direction of flow and vertical downward direction

$K(h)$ = hydraulic conductivity as a function of matric potential

θ = volumetric water content

The system can simulate water movement in either a finite length soil column with uniform or nonuniform conditions, or in a semi-infinite soil

column with uniform initial conditions. For the finite soil column of length L, the initial condition is:

$$h(z,t) = h(z,0) \quad for \quad t = 0 \quad and \quad 0 < z < L \tag{29}$$

Four types of boundary conditions can be employed at the surface of the soil column: constant potential, constant flux, mixed type boundary, and rainfall. The rainfall boundary condition is a specific case of the mixed type boundary where the flux equals to the rainfall rate and the matric potential at the top of the column equals zero. For the finite soil system, the same boundary condition choices are available at the lower boundary except for the rainfall boundary condition.

Movement and degradation of contaminants are simulated using the convection-dispersion equation:

$$\frac{\partial}{\partial t}(\theta C + \rho S) = \frac{\partial}{\partial z}\left(\theta D\left(\frac{\partial C}{\partial z} - qC\right)\right) - \lambda_1 \theta C - \gamma_1 \rho S + \lambda_0 \theta \tag{30}$$

where

C = contaminant concentration dissolved or liquid phase

S = concentration of contaminant in solid phase

D = dispersion coefficient

q = flux of water

ρ = soil bulk density

λ_1 = first order decay in liquid phase

γ_1 = first order decay in solid phase

λ_0 = zero order decay constant in liquid phase

Assuming instantaneous equilibrium adsorption and linear partitioning, $S = \kappa C$, where κ is the linear partition coefficient. Incorporating linear partitioning into Equation 30 yields:

$$\frac{\partial}{\partial t}(\theta R C) = \frac{\partial}{\partial z}\left(\theta D\left(\frac{\partial C}{\partial z} - qC\right)\right) - (\lambda_1 \theta + \gamma_1 \rho \kappa) C + \lambda_0 \theta \tag{31}$$

where $R = 1 + \rho\kappa/\theta$ is the retardation factor for the contaminant in the soil column. CHEMFLO solves Equation 30 coupled with Equation 28 to obtain the dissolved contaminant. The particulate contaminant is estimated from the instantaneous equilibrium adsorption relationship.

Evaluation. The code was able to solve the example cases contained in the database. The example cases demonstrate the capabilities of CHEMFLO and allow the user to apply the different moisture-retention models. The soils database was useful in finding ranges for the fitted parameters of the different soil-moisture models. Though the model is user friendly and fairly fast in solving some typical soil-moisture problems, it can be very slow in solving problems where the moisture content of the

soil is very small. The time steps required to achieve converging solutions can be as small as 10^{-6} hr, where dry conditions exist.

The model was evaluated against the Prill, Johnson, and Morris (1965) experimental column drainage data. The Fresno medium sand fitted parameters were estimated (Figures 7 and 8) using van Genuchten's and Haverkamp's moisture-retention models. Figure 35 shows the water movement simulation against the experimental data. The model performance at the early time periods (1, 2, and 4 hr) are not as good as the later periods (16, 75, and 96 hr). Overall, the model results compared favorable with UNSAT1 and SUTRA, while the input data required were much less than that required by SUTRA and UNSAT1. Figures 36 and 37 show sensitivity analysis on both saturated hydraulic conductivity and time step, respectively. The effect of the time step was not as critical since the largest time step, 1 10^{-3}, was small enough for a stable and converging solution. A smaller time step, 1 10^{-5}, did not improve the simulation. The saturated hydraulic conductivity did not show major effects with changes in the hydraulic conductivity of less than 50 percent (Figure 36).

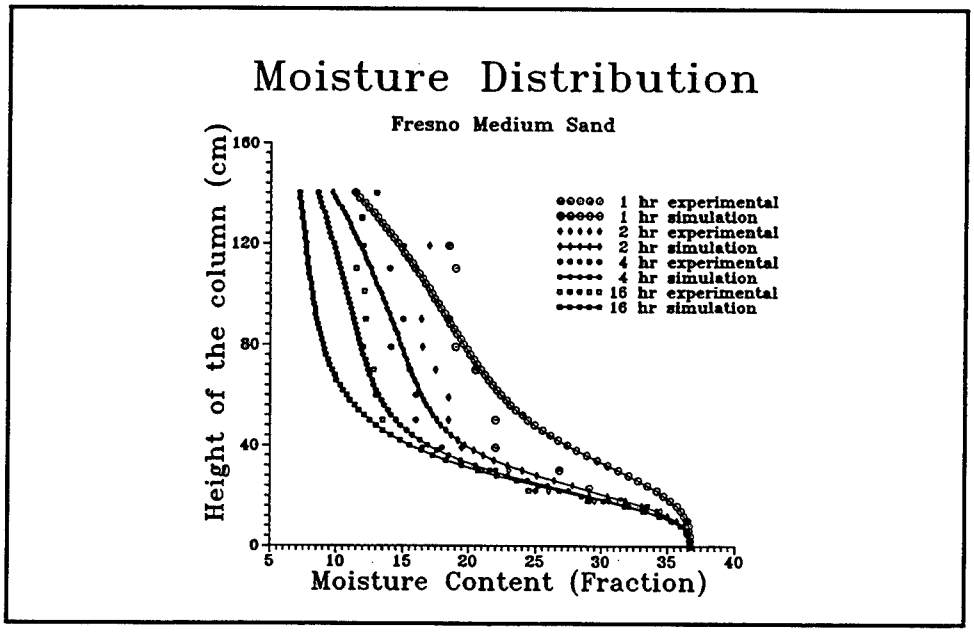

Figure 35. Column drainage simulation, Fresno medium sand

Summary. The CHEMFLO system is very useful and powerful; the model did a very credible job of simulating water movement through a soil column. The software is user friendly, the user's guide is well documented, and the model equations, boundary conditions, as well as the limitations are presented in the documentation. The system is a great teaching and screening tool for fate and transport of contaminants in the vadose (unsaturated zone). CHEMFLO is an appropriate tool when a site has limited amount of data. The model can be used to assist in the application of more complex two- or three-dimensional unsaturated and or coupled groundwater models. Further, CHEMFLO evaluation with data from either a transport experiment or a hypothetical scenario is recommended.

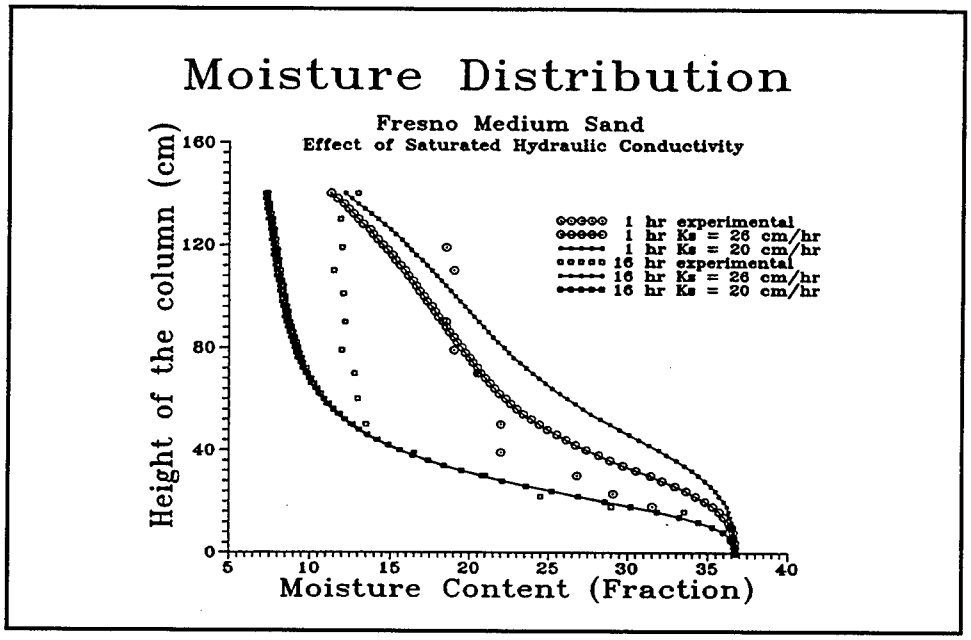

Figure 36. Effect of saturated hydraulic conductivity, Fresno medium sand

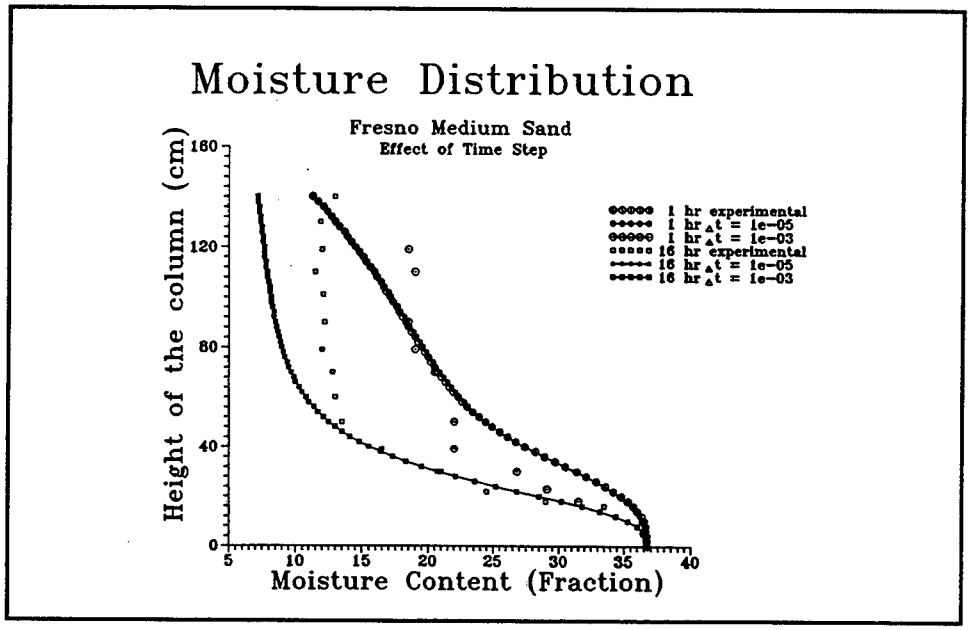

Figure 37. Effect of time step on Fresno medium sand column drainage

One setback is that the system is distributed as a PC executable; thus, no source code is available with the distribution disk.

The transfer of the graphical screens from the display to an attached laser printer did not work. The software Pizzazz Plus was used to capture the screen display and transfer them to the laser printer. Other public domain screen capture programs will probably perform as satisfactorily as Pizazz Plus.

PRZM-2

The Pesticide Root Zone Model, PRZM-2, was developed as a tool for predicting pesticide fate in the crop root and unsaturated zone. The model is supported, updated, and distributed by the Center for Exposure Assessment Modeling (CEAM) at the U.S. EPA Environmental Research Laboratory located in Athens, GA. The model can be obtained free of charge from CEAM's electronic Bulletin Board System (BBS) or by sending the appropriate number of diskettes to CEAM. Obtain information regarding these procedures by telephoning CEAM at (706) 546-3549 or by writing to the following address:

Model Distribution Coordinator
Center for Exposure Assessment Modeling
Environmental Research Laboratory
U.S. Environmental Protection Agency
960 College Station Road
Athens, GA 30606-2720

The PRZM-2 model was originally developed and tested on a Digital Equipment Corporation (DEC) VAX 6310 using VAX VMS FORTRAN-77. The current distribution version of PRZM-2 was built using the Lahey FORTRAN (F77L-EM/32) extended mode FORTRAN compiler Version 5.01. The operation of the PRZM-2 model has the following run time requirements:

- 386 or 486 compatible microcomputer
- MS or PC DOS version 3.30 or higher
- 640K base memory
- 4 MB of extended (XMS) memory
- 4.5 mb free hard disk storage

The PRZM-2 model can also be run on other computers. It has been run on a PRIME 50 Series minicomputer running under PRIMOS, the SUN SPARC station running under UNIX/SUNOS, and the IBM PS/2 Model 8085-071. The model comes complete with an executable file, the FORTRAN source code files, and the make files required to compile, link, and run the task image file PRZM2.EXE. The model does not include a text editor or FORTRAN development tools that would be required to modify the source code for specific applications. User-modified versions of PRZM-2 are not supported by the CEAM. Most applications of the PRZM-2 model will not require program modification. Thus, the user will only need to set up the appropriate input and output data files and run the PRZM2.EXE program.

Overview. PRZM-2 is a management tool that was written to evaluate the effects of the application of pesticides applied for agricultural purposes on water quality. The model is capable of determining the fate of chemicals as they migrate through the crop root and vadose zone. It is also capable of simulating the effects of multiple pesticides and can perform basic exposure assessments. The model was developed at the Environmental Research Laboratory in Athens, GA.

A one-dimensional, dynamic, continuous compartmental model, PRZM-2 was developed by modifying PRZM, Version 1. The modifications to PRZM-1 were necessary to improve the hydrology, soil hydraulics, and solution techniques for the transport equation and to add a stochastic component to the model. One improvement that was made was the addition of the Vadose Zone Flow and Transport Model (VADOFT) module, written to handle flow and transport through the unsaturated zone. Unlike PRZM-1, which assumes the soil drains to field capacity following the addition of water into the root zone, VADOFT allows for variable moisture contents. Thus, in areas where drainage is restricted, PRZM-2 with VADOFT will produce a more realistic simulation than PRZM-1. The PRZM-2 model can be run with or without VADOFT.

The model consists of four main modules: EXESUP, PRZM, VADOFT, and MONTE CARLO. The first of these, EXESUP, is the module that controls the simulation. The user can specify whether or not to run PRZM, VADOFT, or MONTE CARLO for a particular run. The PRZM module controls transport and transformation simulations for the root zone. This module can be run for the entire unsaturated zone if the soil type is one that typically drains to field capacity rapidly following storm events. VADOFT performs transport and transformation simulations for the vadose zone. This is the option that should be used for soils with low hydraulic conductivity values. The last module, MONTE CARLO, if selected will provide the user with uncertainty or risk assessments. This module will provide probabilistic estimates of exposure concentrations by taking into account the variability encountered in natural systems and the uncertainty in system properties and processes. The two major computational modules are PRZM and VADOFT. PRZM provides pollutant fate calculations for the root zone and has the capacity to incorporate the effects of various management practices, and VADOFT is used to calculate transport and fate of the chemicals within the vadose zone. Both of these modules are used for one-dimensional transport. The modules are connected by the use of bridging algorithms that conserve water and solute mass.

Input/output parameters. The operation of the PRZM-2 program requires several input files. The input files include a meteorological file (MET.INP), an execution supervisor file (PRZM2.RUN), a PRZM input file (PRZM.INP), a VADOFT input file (VADOFT.INP), and a MONTE CARLO input file (MC.INP). The first two files, MET.INP and PRZM2.RUN, are required for each run. The other three, PRZM.INP, VADOFT.INP, and MC.INP, are only required if they have been specified as being "on" in the execution file. Of course, at least one of the three must be "on" for the program to run. After a run has been completed, the output file PRZM.OUT is created, and the user can find the information requested for the run in this file. Other files that are created are TIMES.OUT and VADF.OUT. The TIMES.OUT file gives the output information for the time series data requested, and VADOFT.OUT presents simulation times and summaries of cumulative flow and concentration values. The names of the input, output, and scratch files can be changed by editing the PRZM2.RUN file.

A chapter in the PRZM-2 user manual entitled "Parameter Estimation" was written to aid users in estimating input parameters required to run the model. The chapter is well written and includes aid in determining input records for EXESUP, PRZM, and VADOFT modules. By no means does

the chapter provide all possible values for all parameters. It does, however, provide a starting place for these values as well as possible sources of reference. The PRZM-2 manual also provides error messages and warning codes, a variable glossary, and PRZM and VADOFT example input files in the appendixes.

The input files are ASCII files following FORTRAN77 format structure. Each input file consists of several file records. The specific format statements for each record are given in Chapter 4 of the PRZM-2 manual. The manual lists the format parameters for the meteorological (MET.INP), execution supervisor (PRZM2.RUN), PRZM (PRZM.INP), VADOFT (VADF.INP), and MONTE CARLO (MC.INP) input files.

The meteorological file, MET.INP, consists of weather data to be used in the run. It includes information on daily precipitation, pan evaporation, temperature, wind speed, and solar radiation. The global parameters are specified in the PRZM2.RUN file. The information contained within this file specifies the desired modules for the simulation, number of zones to simulate, input and output file names, starting and ending simulation dates, number of chemicals to simulate, weighing parameters between PRZM and VADOFT, and echo and trace levels during execution. Without the meteorological and execution supervisor files, the PRZM-2 program will not run.

The PRZM, VADOFT, and MONTE CARLO input files also consist of formatted records. Each of these input files can be turned "on" or "off" as specified in the PRZM2.RUN file. If a file is turned "on," then it must be defined. Otherwise, it can be omitted. The exception is the VADOFT module; it must be included whenever the vadose zone transport simulation is turned "on" as well as when it is turned "off." A complete description of these input files, as well as the format statements for each file record, can be found in Chapter 4 of the PRZM-2 users manual. These input files are also well documented in the manual.

The user can specify the output frequency. A selection can be made for either daily, monthly, or annual summaries. Predictions in the model are made on a daily basis. Thus, daily time series values for the specified fluxes and storages can be written to sequential files. An additional feature in PRZM-2 is the ability to specify a SNAPSHOT. The SNAPSHOT feature allows the user to obtain the pesticide concentration for each soil compartment at user-specified times during the simulation period. Thus, even if the user has selected monthly or annual output, concentration profiles can still be obtained for any desired day during the run using the SNAPSHOT feature. There is no limit on the number of SNAPSHOTs that can be taken during a simulation.

As previously mentioned, the output file names can be selected by the user in the PRZM2.RUN file. Typically, four output files are created during a simulation: PRZM.OUT, TIMES.OUT, VADOFT.OUT, and MC.OUT. Additional output files created are RESTART.PZM, VFLOW.RST, and VTRANS.RST. These files are used to restart the simulation at the previous simulation termination point. This allows continuation of a simulation without having to repeat the initial run.

The PRZM.OUT file contains information pertaining to both the input and run information. The file first lists the input data used for the run and includes the simulation start and end dates, hydrology and sediment related properties, soil and erosion parameters, crop information, pesticide properties, and soil-horizon data. Basically, this is a tabular summary of all input data. Next, the output that was selected in the PRZM.INP file is given. This can include hydrologic, pesticide flux, and pesticide concentration data in either daily, monthly, or annual form. The TIMES.OUT file contains the time series data for selected parameters. The specific times that data are printed in this file were selected by the user in the PRZM.INP file. A maximum of seven time series plots can be made for each run. Flow and transport output data from the VADOFT module can be found in the VADF.OUT file. This file contains cumulative volumetric storage, inflow volume, outflow volume, mass storage, mass decay, inflow mass, and outflow mass. Once again, the data are printed out at daily, monthly, or annual intervals as specified by the user. Even if a daily or monthly output is selected, the file will still print out annual summaries of cumulative concentration at the end of the file. The MC.OUT file contains information regarding the input and run data. The input data are printed as a summary for the MONTE CARLO run. This includes the number of input parameters being varied, confidence level, and statistical description of each parameter distribution. The output is given as a flux for each chemical based on the statistical description entered by the user.

Evaluation. The current documentation of PRZM-2 has several example files that can be used to test the program. The examples that are given include both input, output, and the execution supervisor files. Two years of weather data are available in the example meteorological input data file (MC.INP). Therefore, the maximum simulation time is limited to 2 years with the example file. The files that are included enable the user to test all three components (PRZM, VADOFT, and MONTE CARLO modules) of the PRZM-2 model. The modules can be run simultaneously or independently.

The time required to run the PRZM-2 program is dependent upon the computer used and the number of modules being run in the program. For example, using a Gateway 2000 4DX2-66V microcomputer (486-66MHz), a time of 7.18 min was recorded running all of the modules simultaneously for the example data set over a 2-year period. However, a time of only 32.79 sec was recorded running the same data set using only the PRZM module. Other factors that affect the run time are the number of years, chemicals, irrigations, horizons, and modules used for the simulation. Using the microcomputer, all of the PRZM-2 example files were run in less than 10 min. While the program is running, the user is provided with a simulation status report that indicates the current step the program is calculating and the percent of the run that is complete. The example data sets supplied with the PRZM-2 program all run correctly without modifications to the files other than the PRZM2.RUN file, which determines the global parameters for each run.

Summary. The PRZM-2 model can be used to simulate pesticide migration through the saturated-unsaturated soil profile in one dimension. The addition of the VADOFT module allows for application of the model to depths greater than that of the crop root zone. After running the example

data sets, the model was able to produce results consistent with physical expectations. The documentation for PRZM-2 is well written, and the model is maintained by the CEAM.

A preprocessor should be added to the model to aid in the creation of input data sets. Currently, the best way to create new input files is to edit the ones that are shipped as examples with the current model. This is a time-consuming process. Also, any characters typed outside of the format field result in errors. Thus, great care must be taken when creating new input files. A preprocessor would enhance the model by providing a better way of creating input files.

The PRZM-2 model is a one-dimensional model and should not be used for field situations such as fields exhibiting a high degree of lateral flow, requiring a two- or three-dimensional model. This may occur in sloping fields with sand over dense clay layers. In such a field, the tendency will be for the water to move laterally as it accumulates at the top of the clay layers. A two-dimensional model allowing for lateral flow would be better suited for this situation than PRZM-2. Selection of the right model is critical in obtaining meaningful results. A good application of PRZM-2 would be in estimating potential pesticide leaching through the vadose zone.

Coupled Unsaturated/Saturated Flow and/or Transport Models

FEMWATER

FEMWATER is a full three-dimensional (3-D) finite element method (FEM) program that models a time-dependent saturated/unsaturated flow of water in porous media. A steady-state solution can also be efficiently obtained as the program has a separate section for this task. Features include the following:

a. *Heterogeneity.* Heterogeneous geologic formations are handled by assigning different hydrogeologic parameters to groups of elements.

b. *Anisotropy.* A full 3 by 3 hydraulic conductivity tensor can be used to model anisotrophy.

c. *Initial conditions.* Initial conditions can be prescribed or obtained from the steady-state solution.

d. *Boundary conditions.* A wide variety of time-dependent boundary conditions are available, including specified head, specified flow, sources and sinks, precipitation and evaporation with ponding options, and automatic time step resetting with sharply varying boundary conditions.

e. Unsaturated flow curves. Pressure head, saturation, relative hydraulic conductivity, and water capacity curves for unsaturated flow can be input in tabular form or computed with analytic functions.

f. *Multiple blocks.* A multiblock definition of the grid and solution of the equations is allowed.

g. *Mass balance.* A mass balance computation over the entire region is done at each time step.

Equations. The governing partial differential equation used in FEMWATER is Richard's Equation

$$\nabla \bullet \left[k_r k_s \bullet (\nabla h + \nabla z) \right] + q = F \frac{\partial h}{\partial t} \tag{32}$$

where

k_r = relative hydraulic conductivity

k_s = saturated hydraulic conductivity tensor

h = pressure head

q = source or sink

t = time

F = water capacity given by

$$F = \frac{d\theta}{dh} \tag{33}$$

where θ is the moisture content. In the saturated zone, F is very small (set to zero in FEMWATER), θ becomes the porosity, and $k_r = 1$. Otherwise, F, θ, and kr are functions of h, making Equation 32 nonlinear.

Evaluation. The performance of the model will now be given. The example problems provided with the documentation were first tested to determine if computed results matched that in the documentation. Results obtained for all three example problems were the same as the output given in the documentation. Three analytical solutions were tested against FEMWATER as discussed below.

1-D vertical flow without gravity. The problem consists of unsaturated vertical flow in a column of sand where the gravity option has been turned off. The problem can also be considered as horizontal flow from one boundary to another. The grid is the same as that given in FEMWATER's documentation (Yeh and Cheng 1994) for the first problem. Each element is 5 m high, giving 164 nodes and 40 elements. Two runs were made with the first being 200 time steps at $\Delta t = 0.05$ day and the second run being for 20 time steps with $\Delta t = 0.5$ day. When the time step is very small, the differences between analytical and computed pressure heads remain stable. However, a large Δt causes a gradual degeneration of results. The first run with 200 time steps took 4 min 48 sec on the Silicon Graphics 4D/320 VGX workstation, and the second run with 20 time steps took 53 sec. The Silicon Graphics 4D/320 VGX runs approximately four times faster than a 486/33MHz PC.

1-D vertical flow with gravity. This problem is very similar to the first problem, except this time the gravity option has been turned on, and the equation for relative hydraulic conductivity has been changed. The grid is the same as that of the first problem, and, as before, $\Delta t = 0.05$ day with 200 time steps. The comparison of analytical and computed pressure heads were again reasonable. However, a gradual loss of symmetry occurred in this example when the tolerance was set at 0.02 but was remedied when it was set to 0.0002. This run with 200 time steps took 4 min 48 sec on the Silicon Graphics 4D/320 VGX workstation.

3-D steady-state flow. This problem consists of steady-state flow in a rectangular region of sand surrounded by clay. Both the sand and clay are initially at zero pressure, but then significant drying occurs on the top boundary of the sand such that now the pressure head is some negative value h_0. The clay keeps the sand at zero pressure on the other boundaries throughout the time period of the analysis. As in the first problem, the gravity term is neglected. The grid is very similar to that given in FEMWATER's documentation for the third example problem. The grid is a rather coarse 21 by 9 by 11 structured grid with $\Delta x = 50$ m, $\Delta y = 50$ m, and $\Delta z = 50$ m except for the last three layers in which $\Delta z = 40$, 30, and 20 m, respectively. The computed pressure heads compared favorably to those determined analytically except where the boundary condition changes abruptly from $h_0 = -30$ to 0 m, requiring a finer mesh in this area. This problem took 4 min. 8 sec. on the Silicon Graphics 4D/320 VGX workstation.

Vauclin's experiment. An experimental study of 2-D transient unsaturated/saturated flow with water table recharge was compared with results obtained from FEMWATER. The problem consists of flow in a homogeneous soil in a tank with an impervious bottom (see Figure 10). An influx of water is provided at the top of the tank with a pool elevation maintained at both side boundaries. The relative hydraulic conductivity versus pressure head curve was found experimentally to be

$$k_r = \frac{A}{A + (-h)^B} \tag{34}$$

where $A = 2.99 \quad 10^6$, and $B = 5.0$. The moisture content equation was also determined experimentally to be

$$\theta = \theta_s \frac{\alpha}{\alpha + (-h)^\beta} \tag{35}$$

where $\theta_s = 0.30$, $\alpha = 40.00$, and $\beta = 2.90$. Thus

$$F = \theta_s \frac{\alpha\beta(-h)^{\beta-1}}{\left[\alpha + (-h)^\beta\right]^2} \tag{36}$$

The grid consists of a 16 by 2 by 16 structured grid with the intervals slightly nonuniform to align with key points. The Δt was set to 0.05 hr and allowed to grow 20 percent per time step until a maximum Δt of 1 hr

was reached. Twenty time steps were run for a total of 8 hr. Because of the nature of the analytical curves of Equations 34-36, which become almost zero in certain regions, FEMWATER had trouble converging to a solution. This was remedied, however, by using the tabular option of the relative hydraulic conductivity, moisture content, and water-capacity curves with the water capacity curve not being allowed to drop lower than a small value of 0.001.

Summary. FEMWATER does an acceptably good job of modeling saturated/unsaturated flow in porous media for the problems tested. Many needed basic features are available to the user, so it is recommended that this model be considered as a viable choice. However, the user may find the input data a bit tedious to prepare without additional tools, especially since this is a 3-D program. In fact, a graphical user interface with grid generation to help prepare the grid and postprocessor capability to visually analyze the results are essential for real-world applications. It is therefore recommended that this model be used in conjunction with such tools. A good choice is the Groundwater Modeling System (GMS) that is being developed for various models, including FEMWATER. Finally, it is recommended that the user select the tabular option for the curves describing the pressure-water content-relative permeability and that it be realized that for nonlinear problems some minor adjustments in the data may be necessary to achieve good results. The model's input, output parameters and documentation are summarized in Figure 38.

FEMWATER	
Version	3-D EPA.
Language	FORTRAN 77.
Platform	486 PC or Unix workstation for small problems. Supercomputer for large problems.
Code	Complete source code provided in ASCII file on floppy disk.
Documentation	Complete report in WordPerfect 5.1 format on floppy disk.
Input	Data file parly in fixed and partly in free-field format. Example problems available on floppy disk.
Output	Results are placed in files. Only information for selected time steps are output.
Memory Requirements	Varies depending on size of problem. Easily adjustable by changing PARAMETER statements in files.

Figure 38. FEMWATER computer details

LEWASTE

LEWASTE is a full 3-D hybrid Lagrangian-Eulerian finite element method (FEM) program that models time-dependent contaminant transport through saturated/unsaturated porous media. A steady-state solution can also be efficiently obtained, as the program has a separate section for this task. Features include the following:

a. *Heterogeneity*. Heterogeneous geologic formations are handled by assigning different soil data to groups of elements.

b. *Anisotropy*. A full 3 by 3 dispersion coefficient tensor can be used to model anisotropy.

c. *Adsorption*. Linear isotherm, nonlinear Freundlich isotherm, and nonlinear Langmuir isotherm adsorption models are available.

d. *Initial conditions*. Initial conditions can be prescribed or obtained from the steady-state solution.

e. *Boundary conditions*. A wide variety of time-dependent boundary conditions are available, including specified concentration, specified flux of contaminant, sources and sinks, variable run-in/flow-out concentration profiles, and automatic time step resetting with sharply varying boundary conditions.

f. *Multiple blocks*. A multiblock definition of the grid and solution of the equations is allowed.

g. *Mass balance*. A mass balance over the entire region is computed at each time step.

Equations. The governing partial differential equation used in LEWASTE is

$$\theta\frac{\partial C}{\partial t} + \rho_b\frac{\partial S}{\partial t} + \mathbf{v}\bullet\nabla C = \nabla\bullet(\theta D\bullet\nabla C) - \lambda(\theta C + \rho_b S) + QC_{in} - QC \tag{37}$$

where

θ = moisture content

C = material concentration in aqueous phase (M/L^3)

ρ_b = bulk density of medium (M/L^3)

S = material concentration in adsorbed phase (M/M)

$\mathbf{v}$ = discharge velocity vector (Darcy Flux, L/T)

D = dispersion coefficient tensor (L^2/T)

λ = decay constant ($1/T$)

Q = source rate of water

C_{in} = material concentration in source

The linear isotherm model for adsorption is

$$S = K_d C \tag{38}$$

where K_d is the partition coefficient. The Langmuir nonlinear isotherm is

$$S = \frac{S_{\max} KC}{1 + KC} \tag{39}$$

where

$S_{\max}$ = maximum concentration allowed
K = coefficient

Finally, the Freundlich nonlinear isotherm is given by

$$S = KC^n \tag{40}$$

where n is the power index.

The ij component of the dispersion coefficient tensor D_{ij} is given by

$$D_{ij} = \frac{1}{\theta}\left[a_T|\nu|\delta_{ij} + (a_L - a_T)\frac{\nu_i \nu_j}{|\nu|}\right] + D^*\tau\delta_{ij} \tag{41}$$

where

a_T = lateral dispersivity
a_L = longitudinal dispersivity
ν_i = i component of ν
D^* = molecular diffusion coefficient
τ = tortuosity
δ_{ij} = Kronecker delta tensor

Evaluation. The example problems provided with the documentation were first tested to determine if computed results matched what was given. Results obtained for all three example problems were the same as the output given in the documentation. Two analytical solutions were tested against LEWASTE as discussed below.

2-D point source (Case 1). A pollutant is continuously injected into a relatively thin aquifer with enough vertical mixing occurring such that it can be treated as a 2-D problem. Water is flowing at a constant velocity in the $+x$ direction. Also, due to symmetry, only the upper half of the problem needs to be solved. A grid of 51 by 11 by 2 was used with $\Delta x = 50$ m, $\Delta y = 50$ m, $\Delta z = 33.5$ m, and $\Delta t = 100$ days (see Table 3 and Figure 4 for more details). Because of the form of the equations used in LEWASTE, the source rate of water Q had to be made small and its input concentration C_{in} large with their overall product being the correct value

of QC_{in} to properly model the analytical problem. With this, the results were quite good. Figure 39 shows a comparison of numerical and analytical results along the bottom of the grid away from the point source for t = 2,800 days. The run with 28 time steps took 20 min on the Silicon Graphics 4D/320 VGX workstation, which runs approximately four times faster than a 486 class PC running at 33 MHz.

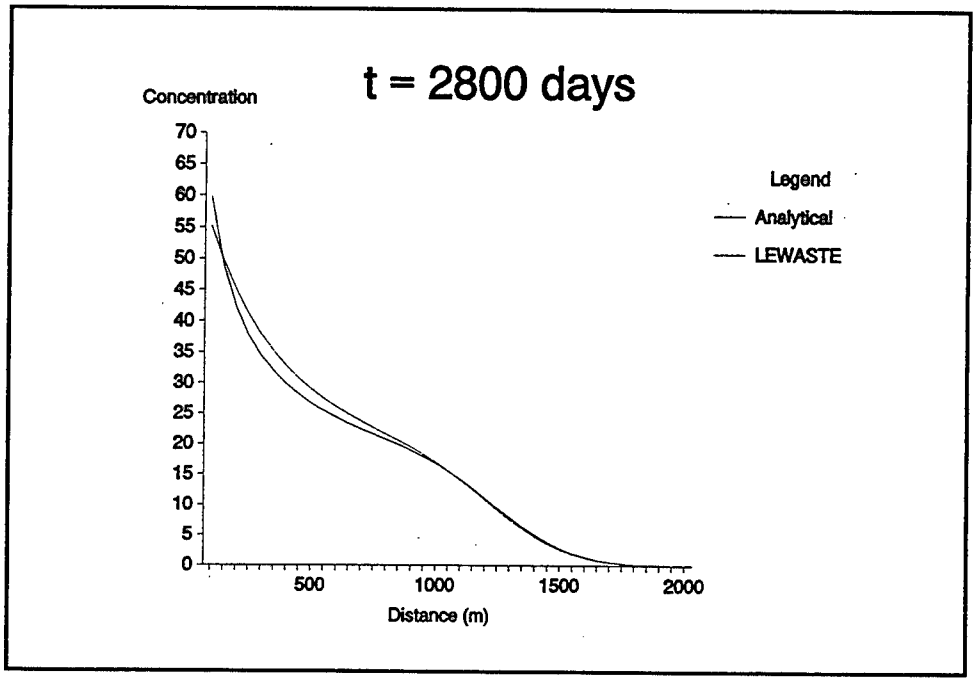

Figure 39. Comparison against analytic solution

3-D problem with time-varying boundary conditions. A full 3-D analytical solution was derived for a problem with time-varying boundary conditions. The problem consists of saturated flow in a rectangular region of sand that is initially clean until a spill occurs on the top of the sand. A concentration C_0 in an s by s square area in the middle and on top of the sand is maintained for a time t_0, and then it decays exponentially with a decay constant α. Water is flowing in the $+x$ direction with a discharge velocity u. However, no contaminant due to dispersion flows to the boundary at $x = a$. Adsorption into the medium of bulk density ρ_b occurs linearly with a distribution coefficient of K_d. The grid is a 21 by 21 by 11 rectangular mesh with $\Delta x = 5$, $\Delta y = 5$, and $\Delta z = 2$. The Δt was first set to 1.0, and 20 time steps were run. The behavior of the solution was understood by looking at a single node through time. Figure 40 plots the numerical and analytical solutions for the time-varying problem. The model captures the trend but overestimates the concentration at the selected node. One explanation for this deviation is that the node selected was too close to the source; with a course grid, the numerical solution will tend to overestimate the concentration. A fine grid would reduce the amount of mass in the element and thus be closer to the analytic solution, which is a point solution. The run with 20 time steps took 1 hr 35 min on the Silicon Graphics 4D/320 VGX workstation. When the relaxation parameter was changed, only 58 min were needed for this run.

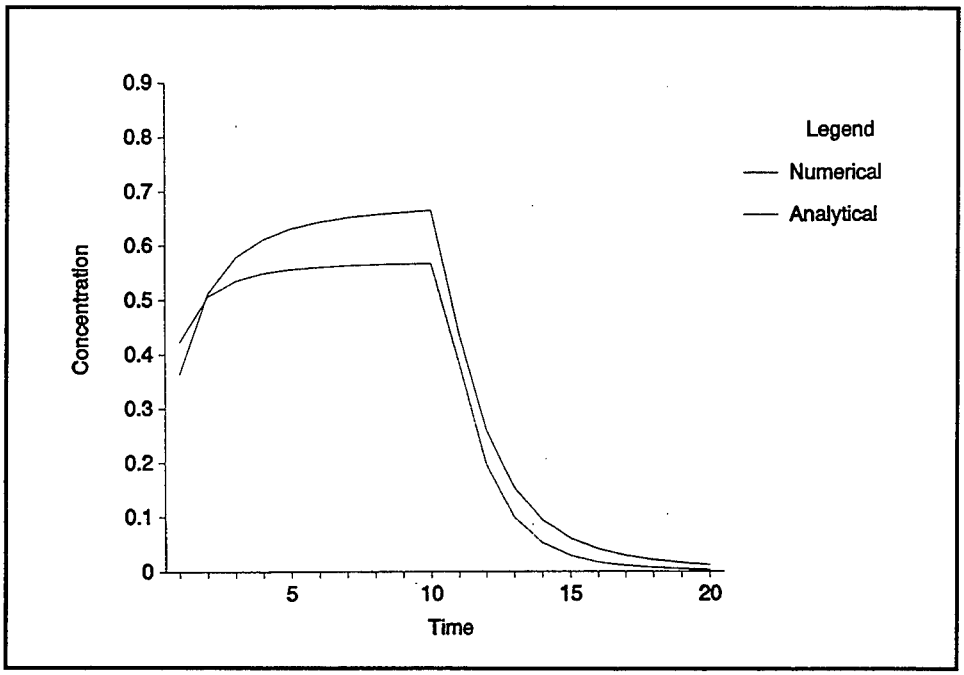

Figure 40. Comparison against 3-D analytic solution

Summary. LEWASTE does an acceptably good job of modeling contaminant transport in porous media for the problems tested. Many needed basic features are available to the user, so it is recommended that this model be considered as a viable choice. However, the user may find the input data a bit tedious to prepare without additional tools, especially since this is a 3-D program. In fact, a graphical user interface with grid generation to help prepare the grid and postprocessor capability to visually analyze the results is essential for real-world applications. It is therefore recommended that this model be used in conjunction with such tools. A good choice is the GMS that is being developed by WES for various models, including LEWASTE. Figure 41 shows the computer code details.

LEWASTE	
Version	3-D EPA.
Language	FORTRAN 77.
Platform	486 PC or Unix workstation for small problems. Supercomputer for large problems.
Code	Complete source code provided in ASCII file on floppy disk.
Documentation	Complete report in WordPerfect 5.1 format on floppy disk.
Input	Data file parly in fixed and partly in free-field format. Example problems available on floppy disk.
Output	Results are placed in files. Only information for selected time steps are output.
Memory Requirements	Varies depending on size of problem. Easily adjustable by changing PARAMETER statements in files.

Figure 41. LEWASTE features

SUTRA

SUTRA (Saturated-Unsaturated TRAnsport) is a computer program that simulates fluid movement and the transport of either energy or dissolved substances in the subsurface environment. Only the fluid movement and solute transport were evaluated under the current effort. The model was developed by the USGS and is distributed by the USGS, Geraghty and Miller, Inc. (G&M), International Ground Water Modeling Center (IGWMC), and Scientific Software Group. The version of SUTRA used in this evaluation was purchased from:

Geraghty and Miller, Inc.
Modeling Group
10700 Parkridge Boulevard
Suite 600
Reston, VA 22091
(703) 758-1200

The current model being distributed by G&M is Version 2.0 and was written by C. I. Voss (1984). The USGS distributes the source code for either a nominal fee or free through the Internet and/or bulletin boards. The user is responsible for the compilation/linkage and execution in the PC environment. IGWMC, G&M, and Scientific Software Group charge a fee for the software to cover the costs of distribution, modification, implementation, and documentation.

Some minor changes were incorporated into the computer code by the G&M staff to take advantage of the personal computer architecture and, in particular, Intel's 80386 CPU. The computer system requirements recommended by G&M are the following:

- 80386 CPU
- 80387 or equivalent math coprocessor
- At least 1MB of extended memory (8MB recommended)
- DOS version 3.3 or higher

The computer model (SUTRA^{386}), as distributed by G&M, includes three executables (1MB, 3MB, and 7MB), three example problems, two utilities to address and tune the personal computer's extended memory, and SUTIL. SUTIL is a utility program that creates XYZ text files compatible with SURFER and other contouring packages. SUTIL also provides a utility that generates portions of the finite-element mesh. Two types of finite-element mesh can be generated with SUTIL, radial and rectangular.

The G&M version of SUTRA was selected because the developers maintain an accountable version of the original code and upgrades to the latest release (Version V-0690-2D) of the program. Shortly after finishing this evaluation, a new release of SUTRA (Version 2.0) became available to users. This review focuses on Version 1.0.

Overview. SUTRA employs a two-dimensional, hybrid finite element and integrated finite difference method to approximate the governing equations. SUTRA simulates fluid density-dependent saturated or unsaturated groundwater flow and either transport of a solute or transport of thermal energy in the groundwater. In simulating solute transport, the solute may be subject to equilibrium adsorption on the porous media, and both first-order and zero-order production or degradation.

SUTRA produces, as the primary calculated result, fluid pressures and either solute concentrations or temperatures, as they vary with time and space. The groundwater system may be either saturated, partly saturated, or completely unsaturated. Fluid density may be constant, or vary as a function of concentration or temperature. The single solute species can be conservative or undergo equilibrium sorption and decay/production. Three equilibrium sorption models are available in SUTRA, linear isotherm, Freundlich, and Langmuir isotherm. SUTRA's dispersion processes include diffusion and two velocity-dependent models: a velocity-dependent dispersion model for anisotropic media and a standard dispersion model for isotropic media. The isotropic model assumes direction-dependent values of longitudinal and transverse dispersivity.

SUTRA is formulated in two spatial dimensions, and simulations can be run either in horizontal (areal) or vertical (cross-sectional) planes for saturated groundwater flow systems. Simulations for unsaturated flow modeling are carried out in the vertical plane; the same is true for variable-density fluid problems. Areal simulation of unsaturated flow and variable-density problems are usually physically unrealistic. In addition, either cylindrical or Cartesian (rectangular) coordinates can be selected. Although SUTRA is two dimensional, a three-dimensional quality is provided in that the thickness of the two-dimensional grid may vary from point to point.

SUTRA is primarily intended for two-dimensional simulation of flow and either solute or energy transport in saturated variable-density systems (Voss 1984). The unsaturated capability of SUTRA was implemented because it is similar to nonlinearities encountered in density-dependent flow and transport problems. Thus unsaturated flow is provided as a convenience to the user, rather than as the primary application tool. SUTRA requires fine spatial and temporal discretization for unsaturated flow and thus is not an economical tool for extensive unsaturated flow modeling (Voss 1984).

Simulations may be employed in one- or two-dimensional problems. Flow and transport simulation can be either steady state or transient. Steady-state solutions are often not appropriate for nonlinear problems (variable density, saturation viscosity, and nonlinear sorption).

SUTRA uses a modular design; thus modifications and additions to the code are fairly straightforward. The design of the code has allowed the development of utilities such as preprocessors and postprocessors and mesh generators. In addition, the modular structure would ease the addition of nonequilibrium sorption, equilibrium chemical reactions, and chemical kinetics.

Input/output parameters. The pressure and water saturations are specified at each node in the problem domain to establish the initial conditions for the flow simulation. Two files, both ASCII and user-generated, provide the input for a SUTRA simulation. They are an initial condition file (pressure and/or concentration) and a mesh, properties, and simulation parameters file. In the input parameters file, the user can select flow, transport, flow and transport, or energy simulation. In addition, the user can select either saturated or coupled saturated-unsaturated flow simulations. The model has a restart option. The model does not have a preprocessor, although the version acquired from G&M included a postprocessor that creates an output file compatible with SURFER.

Equations. Flow simulation in SUTRA is a calculation of how the amount of the fluid mass contained within the void spaces of the fluid matrix changes with time (Voss 1984). The flow equation solved by SUTRA is Equation 15. The fluid density is assumed to be a function of pressure (weak), temperature, and solute concentration. For solute transport, the concentration dependence is of the form:

$$\rho = \rho_0 + \frac{\partial \rho}{\partial C}(C - C_0) \tag{42}$$

For unsaturated flow, SUTRA requires a capillary-pressure saturation relationship to describe hydraulic conductivity and pressure saturation. The functions have to be supplied by the users; forms include those in Figures 2 and 3. The model includes the van Genuchten relationship.

Solute transport is described by Equation 16. Since fluid properties are functions of solute concentration, an interactive approach is used within each time step to resolve the nonlinear coefficients in the fluid flow and solute transport equations.

Numerical methods. SUTRA includes an optional numerical method based on asymmetric finite element weighing functions that results in "upstream weighing" of advective transport and unsaturated fluid flux terms (Voss 1984). In simulating transport problems, upstream weighing is generally discouraged. SUTRA numerical algorithms are not specialized for the nonlinearities of unsaturated flow.

The model uses quadrilateral elements with four corner nodes to allow the simulation of irregular regions. Coefficients and material properties can vary throughout the mesh. Either Cartesian or radial coordinates may be selected.

Evaluation. SUTRA's evaluation included the three example problems included with the documentation. The model solved the example problems without any difficulty. In addition to the example problems, the model was evaluated against Vauclin's experimental data (Vauclin, Khanji, and Vachaud 1979) and against the saturated analytical solutions of Cases 1, 2, and 3. The model performed satisfactorily. The choice the of coordinate system in SUTRA was useful in solving the test Case 3.

Vauclin's experiment. The model was run with the data from Vauclin described in Figures 12-17. The two-dimensional grid was constructed,

and the saturation models described in Figures 2 and 3 were used in the simulations. The van Genuchten model had difficulties with the experimental data at low-moisture levels. The pressure (suction) at low-moisture content was very large (negative numbers) and thus created some arithmetic underflow/overflow problems. The Campbell relationship was used with the Vauclin data, and the results are shown in Figure 42. The Campbell model does not predict as large negative pressures as van Genuchten's for those periods of low-moisture content. The results are comparable with those from VS2DT and FEMWATER.

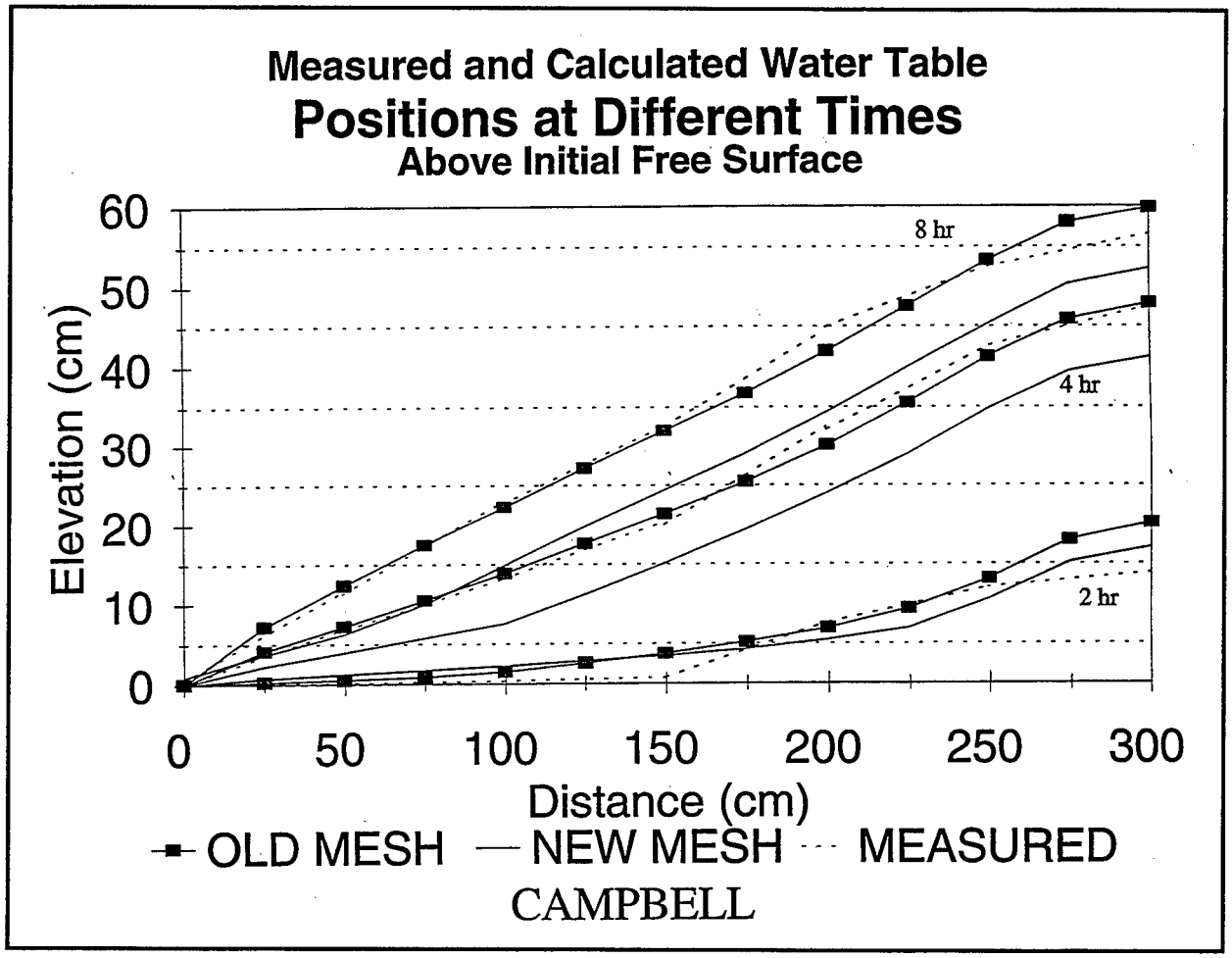

Figure 42. Water table elevation: Experimental and simulated results

Summary. The model evaluation was satisfactory; SUTRA is recommended for further evaluation. The model was modified to include the four moisture relationships described in Figures 2 and 3. SUTRA's advantages are as follows: the code's maturity (released in 1984 and modified in 1992); the code's versatility (saturated, unsaturated, energy, temperature simulations); and ease of modification.

VS2DT

VS2DT is a two-dimensional (vertical cross section, x-z) or axially symmetric three-dimensional (cylinder, r-z) computer code that can be used to solve problems of flow and solute transport in variably saturated porous media. The porous medium may be heterogeneous and anisotropic, but the directions of flow must coincide with the axes of the coordinate system. VS2DT is an extension of the VS2D program, which was developed by USGS to solve flow equations for variably saturated porous media. At present, there is no documentation that describes flow capabilities in VS2DT. Therefore, the user must review VS2D documentation for the aspects of VS2DT. The flow equation used in VS2DT is based on the conservation of mass and Darcy's equation. The flow boundary conditions may be prescribed as known pressure heads, known fluxes, evaporation from surface, plant transpiration, and/or seepage face boundaries. Flow source and/or sink terms such as injection wells or pumping wells also are included in the solution. The flow and mass transport equations were solved numerically using central finite differences about grid-block boundaries. Time derivatives are approximated by a fully implicit backward finite difference scheme. The effects of advection, dispersion, adsorption, and ion exchange on a chemical can be simulated by VS2DT. The decay of solute mass in the solid phase is also incorporated in the mass transport solution.

Both VS2D and VS2DT programs and their documentation are available from the Geraghty and Miller Modeling Group. The available version of VS2DT from Geraghty and Miller is compiled with the Lahey F77L-EM/32 FORTRAN Compiler. A minimum of system requirements for running VS2DT is given as as follows:

- 80386 CPU.
- 80387 or equivalent math coprocessor.
- At least 1 MB of extended memory.
- DOS version 3.3 or higher.

Equations for flow. The flow equation used in VS2DT (or VS2D) is a combination of a continuity equation and Darcy's flow equation. The equations describe the movement of water under isothermal and isohaline conditions. The governing flow equation is nonlinear and was solved numerically using a block-centered regular finite-difference scheme for spatial discretization and a backward finite difference method for temporal discretization. The nonlinear, discretized flow equation is solved numerically using a modified Newton-Raphson iterative technique.

The flow module of VS2DT provides the solution for total hydraulic head. The total hydraulic head is defined as the sum of pressure head and elevation potential. Below the water table, the pressure head is proportional to the weight of the overlying water. Above the water table, water is held in porous media by adsorptive and capillary forces. Therefore, the pressure head in the unsaturated zone is calculated using a capillary pressure formulation. The capillary-rise equation is applied to the movement of water into relatively coarse-grained materials such as silt, sand, and

gravel. In media containing a large fraction of clay-size material, adsorption forces may be more significant than capillary forces.

The elevation potential is a measure of the gravitational potential resulting from a position relative to an arbitrary datum. In VS2DT, the datum is located at or above the land surface; therefore, the elevation potential is always negative.

Initial and boundary conditions. The initial flow conditions in VS2DT can be specified in terms of the initial pressure head or the initial volumetric-moisture content. The program computes the initial condition for the total pressure head from these input parameters.

When the moisture content is used for the initial condition, the user must prescribe a relationship between pressure head and moisture content. The water-retention relationship can be coded in a predefined function program of VSTHU or VSTHNV. VSTHU is read in VS2DT and provides volumetric moisture content as a function of pressure head. VSTHNV, also read in VS2DT, defines pressure head as a function of volumetric moisture content.

Another type of initial condition is the equilibrium profile, in which the pressure potential is in equilibrium with the elevation potential above the water table. VS2D has an option to automatically compute pressure heads to provide the equilibrium profile. The user can specify a constant minimum pressure head to replace the upper part of the equilibrium profile. For more information, the reader is referred to the VS2DT user's manual.

Flow boundary conditions in VS2DT can be specified either as flux, pressure head, or total otentiometric head (pressure head + elevation head). The values of infiltration, evaporation, and discharge through seepage faces also can be specified as boundary conditions.

Infiltration and ponding. The effect of infiltration or sprinkler irrigation is coded as a two-stage process. In the first stage, water enters the system at an applied rate until the conductive and sorptive capacity of the medium is exceeded. After the capacities are exceeded, water ponds on the surface, and the infiltration rate decreases asymptotically to a rate equal to the saturated hydraulic conductivity of the medium. VS2DT infiltration options are as follows:

a. Specified flux boundary conditions (PFDUM) at the surface equal to the infiltration rate prior to the time ponding occurs, t_{pond}.

b. Specified pressure boundary conditions (POND) at the surface equal to the maximum height of ponding after ponding occurs. The ponding time, t_{pond}, is determined by the model during simulation.

Evaporation and evapotranspiration. Evaporation is the amount of soil moisture that escapes from the soil surface due to surface and ambient atmospheric conditions. The evaporation process is formulated as a two-stage process. In the first stage, evaporation occurs when the land surface is wet; thus liquid leaves the system at a rate equal to the atmosphere's evaporation demand. The evaporation rate is referred in VS2DT

as potential evaporation rate (PEV). The second stage starts after the source of water to the surface has diminished.

The two-stage evaporation process can be expressed by two boundary conditions at land surface:

a. Specified surface boundary flux equal to the potential evaporation demand, until there is not enough water to meet this demand.

b. Specified surface boundary flux as function of the pressure potential gradient between the soil and the atmosphere.

VS2DT handles boundary condition transition for the two-stage process. Potential evaporation in VS2DT is implemented using an empirical formulation. The value is changed with time in a user-defined manner. Details of numerical implementation are given in the VS2DT user's manual.

Transpiration is the amount of soil moisture that can be removed by plant-root extraction. Transpiration is treated in VS2DT as a sink term. The rate of water withdrawal is formulated using an empirical equation. To simulate a problem with evapotranspiration, the logical variable (ETSIM) in the input file must be set to TRUE. In addition, values for the variables, PET (potential transpiration), HROOT (minimum pressure in roots), RTDPTH (the depth of rooting), RTBOT (the root activity at the bottom of the root zone), and RTTOP (the root activity at land surface) must be specified. Refer to the VS2DT user's manual for further information.

Seepage faces and sink terms. Seepage faces are boundaries where a phreatic surface of a flow domain terminates on a land surface. At a seepage face boundary, the total pressure head is equal to the potential elevation head. Examples of seepage faces are boundaries along stream banks, spring discharge zones, and well bores that tap unconfined aquifers. The upper limit of a seepage face is determined by the location of the water table, which is unknown. The location of this intersection is part of the solution. Therefore, determining the seepage face boundaries is a nonlinear problem. VS2DT solves seepage face problems iteratively.

Flow source and sink terms can be specified in VS2DT. Source terms include injection wells (L^3/T) and drip-irrigation (L/T) devices; sink terms include pumping wells (L^3/T) and suction lysimeters (L/T). Evapotranspiration or plant-root extraction can also be treated in VS2DT as sink terms.

Equations for solute transport. The formulation used for solute transport modules in VS2DT includes an advection term, a hydrodynamic dispersion (mechanical + molecular) term, and source/sink terms. Source/sink terms include a fluid source/or sink, adsorption, decay, and ion-exchange reactions in solution.

The decay of a solute (such as radioactive decay) is incorporated by a linear relationship between the sink term and the concentration of solute. The solute adsorption from the water phase onto the solid phase is given in a special case of the Freundlich isotherm (n = 1) as a constant ratio between the solid phase and water (liquid) phase, linear partition. For non-ionic organic chemicals, this ratio, K, represents adsorption onto organic

matter in soils. Nonlinear adsorption between the solid and liquid phases is given by the Langmuir and Freundlich isotherms. Ion exchange is another type of reaction that has been included in VS2DT. Four types of ion exchange are coded in VS2DT: monovalent-monovalent exchange (such as the exchange of sodium and potassium), divalent-divalent exchange (such as the exchange of calcium and strontium), monovalent-divalent exchange (such as the exchange of sodium with calcium), and divalent-monovalent exchange (such as the exchange of calcium with sodium). Detailed information on adsorption and ion exchange can be found in books such as Feeter (1993).

Initial and boundary conditions. Initial conditions for solute concentration can be specified either as a fixed constant concentration in the main input file or read from a user-defined file (unit IU).

Two types of solute boundary conditions can be specified in VS2DT, constant concentration and mass flux condition. In addition, if a fluid source exists, the concentration entering the system must be specified. The evaporation boundary condition is treated in a unique form, different from other boundary conditions. Evaporating water is assumed free of chemical contamination.

Sources and sinks. Six source/sink options are available in VS2DT: Freundlich isotherm, Langmuir isotherm, and four ion-exchange options defined previously. Linear adsorption can be modeled using the Freundlich isotherm with the exponent set 1. The present version of VS2DT is set up to use the Langmuir isotherm. The other five options are not active. To activate each option, the user needs to remove comment (*C*) parameters in front of the selected option in the function subprogram, VTRET, and recompile and load the programs. In addition, proper flag and input parameters must be specified in the input file. Only one option can be used per simulation. In other words, for each option simulation, VTRET must be changed; the programs need to be compiled and linked. Variable adsorption rate and ion exchange for different texture classes of soil are possible by varying the coefficients.

Input/output parameters. Data for VS2DT simulation are read from a user-created ASCII (text) input file. The numerical values of parameters are read as free-formatted input. Entry of data using the form n*d results in n values of d being read into the program. Each event (e.g., infiltration event) must be ended by 999999 /; the end of the input record is also invoked by 999999 /.

A successful simulation of VS2DT requires the definition of input parameters and flags in proper order. An easy way to create an input file is to modify an existing input file by adding or removing parameters required for the specific problem.

VS2DT creates a main output file and other files that store individual output parameters as requested in the input file. The output file names are assigned by the user.

Evaluation. Example data sets included with the model ran without difficulties. In addition, two problems were selected for further testing.

Vauclin's experiment defined in the test cases section was used in the evaluation of the variable saturation formulations of VS2DT. A second test case, an injection well into a radial flow domain, was selected to evaluate both the saturated formulations and the radial coordinate system.

Variably saturated flow using tabulated initial pressure condition. In this example, VS2DT is used to simulate flow in a variably saturated soil system reported by Vauclin, Khanji, and Vachaud (1979). The domain is a soil slab 3 m long and 2 m high and 5 cm thick (Figure 10). The soil was packed as homogeneously as possible with average bulk density of 1.57 g/cm^3. At one end of the slab, a constant head reservoir was located. The water table was imposed at 135 cm (depth). A constant flux at the surface, q = 14.8 cm/hr, was applied over a width of 50 cm. The saturated hydraulic conductivity of the fine sand was 35 cm/hr. Tabulated initial pressure heads were used in this simulation (Figure 12). Simulation results and comparison against experimental data are shown in Figures 43 and 44.

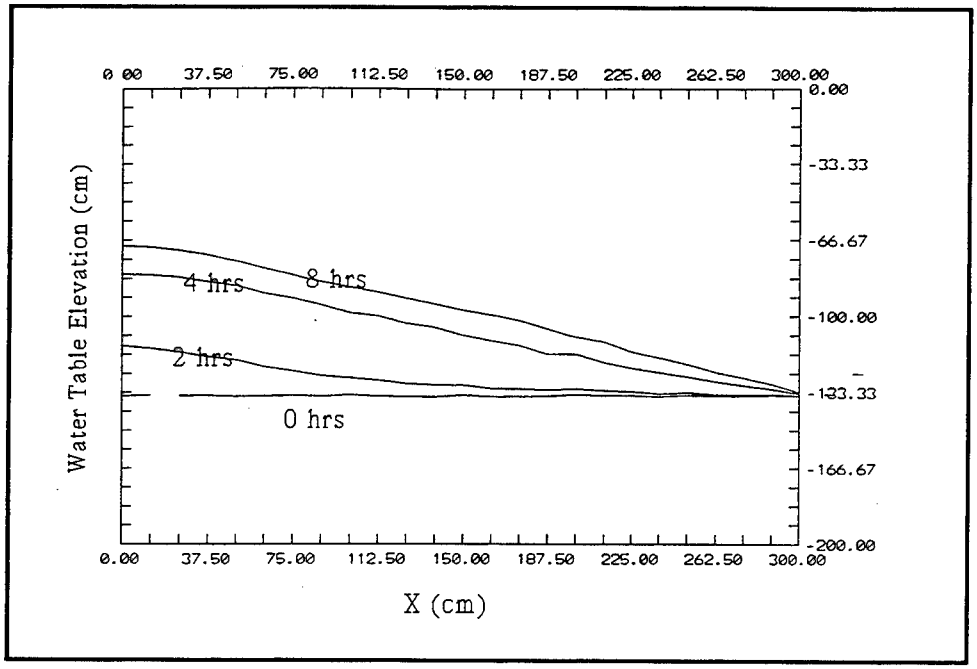

Figure 43. Water table simulation

Injecting a conservative tracer in a radial flow system. In this example, fluid is injected into a fully saturated confined aquifer. Initially, the solute concentration in the aquifer is 0. The injected water has the concentration of 1. A variable spacing in vertical and horizontal directions were used. The hydraulic conductivity, the longitudinal, and the transverse dispersivity are set to K = 0.36 m/hr, α_L = 10.0 m, and α_T = 0.0 m. A pumping period of 2,200 hr was simulated. Flow boundaries consisted of a constant flux of 225 m^3/hr at the injection well and a fixed head of 10.0 m at the radial boundary. VS2DT results are shown in Figure 45. Model simulation and analytic solution fall on top of each other.

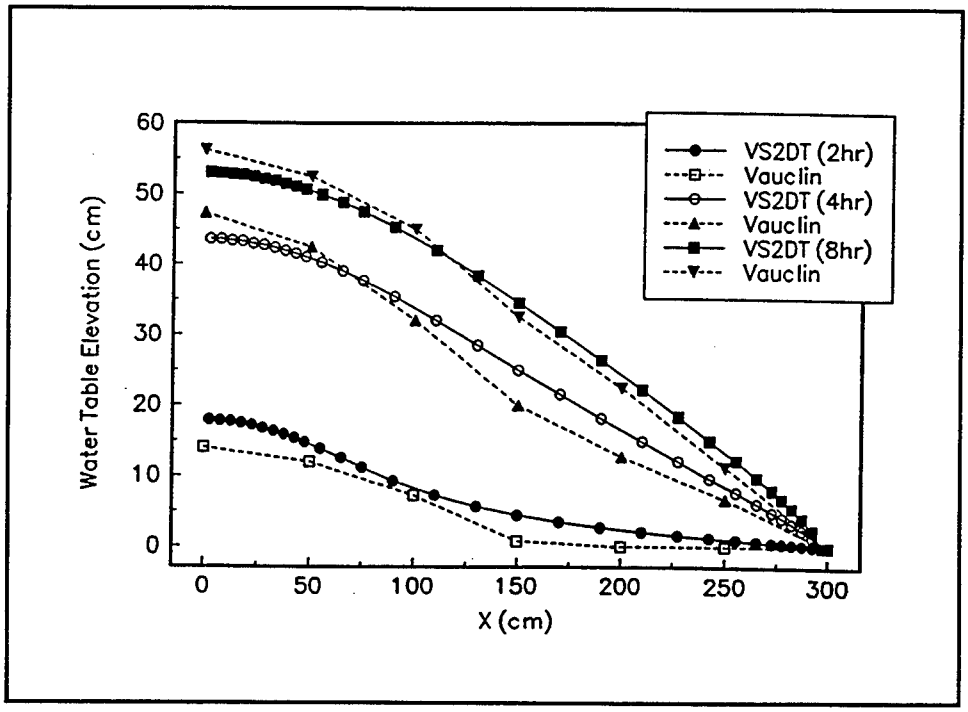

Figure 44. Simulated water table versus experimental data (Vauclin, Khanji, and Vachaud 1979)

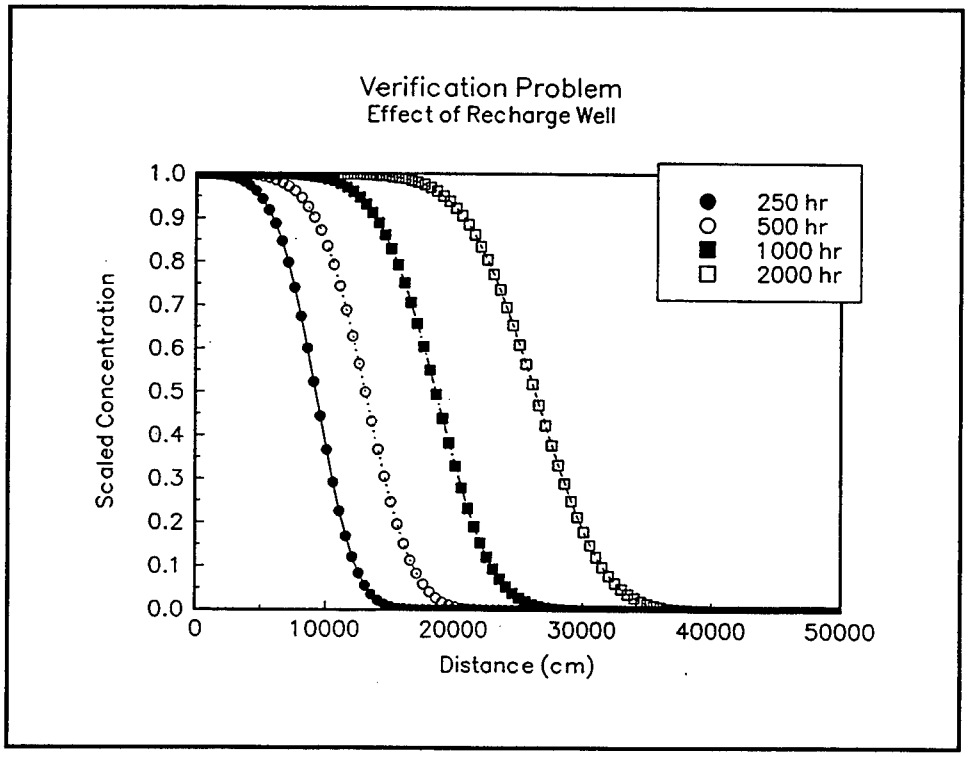

Figure 45. Injection well in radial flow domain

Summary. In general, VS2DT performed satisfactorily to problems provided in the user's manual. In addition, the program was compared with published laboratory measurements and analytic solution. Results of VS2DT simulations were in good agreement with the published data. The example problems involved physical processes such as infiltration, evaporation, evapotranspiration, and injection wells in radial flow. The soil conditions in these examples changed from fully saturated, fully unsaturated to mixed unsaturated-saturated zone conditions. For the unsaturated-saturated example problem, smaller time steps and spatial discretization were required to provide convergence and a stable solution. Other options, such as ion exchange and adsorption, available in VS2DT were not evaluated.

Although VS2DT can be used for one-dimensional (x or z coordinate system) problems, the numerical solution in the Cartesian coordinate system is always two-dimensional. For one-dimensional vertical problems, the horizontal dimension is used in calculations; however, the effect of the horizontal dimension on the results will be negligible due to the lack of horizontal loads and flow. The vertical saturated hydraulic conductivity in VS2DT is always calculated from the input horizontal saturated hydraulic conductivity. The user must always specify the value of the horizontal hydraulic conductivity and a coefficient named ANIZ in the input file. The value of vertical hydraulic conductivity is calculated by the computer code as $K_z = ANIZ * K_x$, where K_z and K_x are the vertical and the horizontal hydraulic conductivity, respectively. The value of initial unsaturated hydraulic conductivity depends on the initial pressure head. Therefore, it is obvious that correct initial pressure head provides a more accurate solution.

In VS2DT, intercell average relative hydraulic conductivities are calculated using either geometric mean or a weighted arithmetic mean. Geometric mean may produce more accurate simulation and should be used whenever possible. The geometric mean option is invoked by inputting WUS = 0 in the input file. In some cases, this option may create numerical oscillation. For these cases, other options may be used. Set WUS = 0.5 for the usual arithmetic mean or WUS = 1 for full upstream weighing. The selection of WUS is important because the value of WUS affects both the accuracy and computational time. An optimum value of WUS for a specific problem is obtained by trial and error, knowing that the value of WUS ranges between 0 and 1.

Other important input parameters are HMAX and EPS. HMAX is a user-defined damping factor used in solution of the final matrix equations. The value of HMAX is recommended to vary between 0.2 and 1.1. A value of 0.7 is given as optimal to obtain reasonable accuracy. To obtain convergence, sometimes a value of 0.3 should to be used. EPS is an error tolerance for the residual of total head.

VS2DT has four options for specifying the relationship between pressure head and water content. These options are a user-defined or measured value, the Brooks-Corey equation, the Haverkamp equation, and the van Genuchten formulation. All options were tested using the default parameters coded in VS2DT. The user-defined or tabulated option for pressure head-water content did not work correctly. Minor adjustments were required in

the main program to read initial pressure head, and major changes were performed in other subprograms for correcting this problem. The table look-up subroutine interpolation algorithm did not perform adequately. Therefore, for the example problem, modifications included fitting the relationships into some arbitrary functions and coding the functions into the subroutine (TB.FOR).

The saturation, using van Genuchten option, is calculated without including the value of residual saturation. However, the residual saturation is used in calculation of the water content. For small values of the residual content, the present form of the van Genuchten subprogram does not create significant errors. But for higher values of the residual saturation, this option may create major errors. This can be corrected by including the residual saturation content in saturation calculation (subprogram VG.FOR).

The fluid density in VS2DT is fixed at 1.0 g/cm^3. Hence, all other parameters must be input in units of grams and centimeters; the time can be in seconds, minutes, hours, etc.

For infiltration problems, the amount of ponding should be included in the input file. If the user does not know whether ponding may occur, a value of zero should be used. If ponding occurs during the simulation, the program informs the user where ponding occurs. Then, the user may change the ponding value from zero to an arbitrary number.

Multiphase Flow and Transport Models—MOFAT and MOTRANS

MOFAT is a two-dimensional (vertical), finite element model for coupled, multiphase (≤3) flow and multicomponent (≤5) transport in porous media. Media properties, flow and transport options, and model features include the following:

- *Flow Conditions*: MOFAT simulates the multiphase flow of water, oil, and/or gas in the vertical plane in either Cartesian (x-z) or radial (r-z) coordinates. Flow conditions may be steady state or transient, unconfined or confined. Isothermal, incompressible (storativity neglected) flow of each phase is described as a function of relative phase density and viscosity, pressure gradients, and saturation-dependent permeability. Three-phase permeability—saturation—capillary pressure constitutive relations (K_p-S_p-P_c, where p = water, oil, or air) are defined using an extended (scaled) van Genuchten model. Gas phase flow may be considered explicitly or assumed to be negligible (atmospheric pressure). Multicomponent phase properties are estimated as weighted averages of pure component properties for density, viscosity, interfacial, and/or surface tensions.

- *Porous Media Conditions*: Up to 10 material types may be specified with unique porosity, anisotropic intrinsic permeability, and van Genuchten model parameters (α and n). The use of linear rectangular elements (i.e., intraelement dimensions are uniform) prevents easy

discretization of irregular hydrogeologic units, but such may be approximated with a stepped distribution of material types. The porous medium is assumed incompressible.

- *Transport Processes*: MOFAT solves an advection-dispersion equation (see below) alternately with the flow equations (weak back-coupling assumption) for up to five noninteracting components and one inert component (as a carrier). Hydrodynamic dispersion, molecular diffusion, NAPL dissolution, volatilization, adsorption (equilibrium of first-order kinetic mass transfer), and first-order decay are also simulated. Mass transfer processes (dissolution, sorption) may be described by equilibrium partitioning or first-order kinetics.

- *Mass Balance Calculations*: Mass balances per se (mass in versus mass out) are not calculated. Total oil and water volumes are tracked and output for all simulations. Global mass totals for each constituent in each phase is output for transport simulations.

- *Initial Conditions* (IC): Spatially variable, initial conditions may be defined for water and oil heads (water-equivalent) and solute concentrations. Initial aqueous phase concentrations may be input as spatially variable or as a specific value in the presence of non-zero NAPL saturation. Equilibrium compositions of the oil and air phases are set by the defined partitioning coefficients.

- *Boundary Conditions* (BC): Type-1 (constant head or concentration; Dirichlet), Type-2 (specified phase volumetric or mass flux; Neumann), and/or Type-3 (specified volumetric phase flux and concentration) boundary conditions may be specified for flow and mass transport for each fluid phase and component. A zero-flux BC (a Type-2) is the default condition for flow and transport. Up to 100 time-dependent BCs (total Type-1 and -2) each with up to four linear subschedules may be defined. BCs can also be redefined at the initiation of a restart problem. Injection or withdrawal wells may be defined by imposing appropriate BCs at selected nodes

- *Numerical Methods*: Governing equations are solved by an upstream-weighted finite element scheme. A Newton-Raphson technique is utilized for solving nonlinear integrations in flow analyses. Linear quadrilateral elements are used. An adaptive solution domain is developed to focus simulation on oil flow regions.

- *Miscellaneous Features*: Simulations may be broken into a series of restart problems, i.e., the final output of one simulation is used as the initial conditions for the next simulation, permitting the user to respecify boundary conditions and numerous other parameters. In addition to explicit time limits, simulation durations may be defined in terms of global change in volume of any fluid phase, e.g., a spill of a finite volume of NAPL into the system.

- *Background*: MOFAT was developed at the Virginia Polytechnical Institute and State University, Blacksburg, VA, for the U.S. Environmental Protection Agency, Office of Research and Development, R.S. Kerr Environmental Research Laboratory (RSKERL), Ada, OK.

Source codes for MOFAT (FORTRAN) and PREMOF (Basic), multiple compiled versions of MOFAT (Lahey), and documentation (Katyal, Kaluarachchi, and Parker 1991) are available from the Center for Modeling Support (CMoS) at the RSKERL. The MOFAT (Version 1.0) obtained from CMoS is evaluated here without modification.

Input/output parameters

MOFAT has a menu-driven preprocessor, PREMOF, but no postprocessor. I/O files are formatted ASCII files. Any consistent metric units may be used: length in meters or centimeters, mass in milligrams, grams or kilograms, and time in days. Standard requisite input includes the following: grid geometry, initial and boundary conditions (e.g., $H_{p(w)}$, $C_{\alpha p}$), and control parameters for time (e.g., duration, initial and maximum time steps), integration, convergence, or upstream weighting.

Each material type (≤10) requires input parameters for porosity (ϕ), hydraulic conductivities (K_x, K_z, or K_r), van Genuchten (VG) model parameters (α, n), residual water saturation (S_m), and maximum residual oil saturation (S_{or}). The NAPL mixture specific gravity (ρ_{ro}) and viscosity (η_{ro}) are specified and constant. Surface tension (ST; σ_w, σ_o) and interfacial tension (IFT; σ_{ow}) are accounted for indirectly in the required VG model scaling parameters, which may be estimated as $\beta_{ao} = \sigma w/\sigma_w$, and $\beta_{ow} = \sigma_w/\sigma_{ow}$. Katyal, Kaluarachchi, and Parker (1991) recommend limits on the scaling parameters to avoid "numerical difficulties."

Transport simulations require additional input including the following: initial and boundary conditions for the water phase only, the density of each pure NAPL constituent (ρ_α), dispersivities (α_L and α_T), partitioning coefficients (equilibrium or first-order kinetic mass transfer), component molecular diffusion coefficients in water, oil, and air ($D_{\alpha w}$, $D_{\alpha o}$, $D_{\alpha a}$, respectively), and first-order decay coefficients in each phase (including solid). Initial oil phase compositions are calculated based on inputs for the equilibrium aqueous phase concentrations and the partitioning coefficient for each constituent. The oil-water equilibrium partitioning coefficient ($T_{\alpha o}$) is Raoult's constant; the air-water coefficient ($T_{\alpha a}$) is based on the dimensionless Henry's constant (H_α). The solid-water partitioning coefficient is a simple linear coefficient, $T_{\alpha o}$. First-order, kinetic coefficients for nonequilibrium mass transfer ($k_\alpha 12$) may be specified for oil-water, oil-air, and water-air partitioning.

Output includes nodal saturations, heads, phase-flow velocities, and the composition (mass/volume) for each phase, as well as an echoing of simulation parameters, material properties, and mesh information. The user may regulate to a limited degree the type and frequency of output. The user may specify a subset of nodes from which output is desired. Pure components are presumed to be liquid (e.g., the need for IFT and ST); if one or more of the NAPL constituents is solid at ambient conditions, approximations would be required. Output does not include spatial variation in phase density.

Simulations are typically carried out in a series of stages, the output of one stage linked to the subsequent stage via a restart or "auxiliary" file. This approach is adopted to more efficiently simulate very different phenomena such as NAPL infiltration into the vadose zone, NAPL dispersal through the subsurface, and the generation of solute and/or vapor plumes. Each stage may involve unique boundary conditions and stability requirements (recommendations).

Equations

MOFAT simulates the transient or steady-state, vertical-plane flow of incompressible water and NAPL and compressible gas through nondeformable porous media. The flow equations in Cartesian coordinates are (Katyal, Kaluarachchi, and Parker 1991):

$$\phi\frac{\partial S_w}{\partial t} = \frac{\partial}{\partial x_i}\left[K_{wij}\left(\frac{\partial h_w}{\partial x_j} + \rho_{rw}u_j\right)\right] + \frac{R_w}{\rho_w} \qquad (a)$$

$$\phi\frac{\partial S_o}{\partial t} = \frac{\partial}{\partial x_i}\left[K_{oij}\left(\frac{\partial h_o}{\partial x_j} + \rho_{ro}u_j\right)\right] + \frac{R_o}{\rho_o} \qquad (b) \quad (43)$$

$$\phi\frac{\partial \rho_a S_a}{\partial t} = \frac{\partial}{\partial x_i}\left[\rho_a K_{aij}\left(\frac{\partial h_a}{\partial x_j} + \rho_{ra}u_j\right)\right] + R_a \qquad (c)$$

where

ϕ = porosity

S_p = saturation of phase p (w = water, o = oil or NAPL, and a = air)

t = time

K_{pij} = conductivity tensor $[L{\cdot}T^{-1}]$ for phase p in Cartesian coordinates i,j (x,z)

Phase p pressure heads, h_p $[L]$, are expressed in water-equivalent terms: $h_a \equiv P_p/\left(g\rho_w^*\right)$, where P_p is phase p pressure, g is gravitational acceleration $[L{\cdot}T^{-2}]$, and ρ_w^* is pure water density standard $[M{\cdot}L^{-3}]$. Relative phase density, $\rho_{rp}\left(\equiv\rho_p/\rho_w^*\right)$, is the ratio of the phase density, ρ_p, to the reference density of water, i.e., ρ_{rp} is the specific gravity of phase p. The unit gravitational vector, $u_j \equiv \partial z/\partial x_j$, is measured positively upward. R_p is the net mass transfer per unit bulk volume $[M{\cdot}L^{-3}{\cdot}T^{-1}]$ into (+) or out of (–) phase p.

Phase conductivities are described in terms of relative conductivities (K_{rp}; relative to fully water-saturated conductivity), which are nonlinear functions of phase pressures or saturations. The van Genuchten (1980) model (VG) is a commonly utilized constitutive equation describing the relationship between phase permeabilities or conductivities (K_p), saturations (S_p), and capillary pressures (P_c) in a two-phase system. Parameters for the VG model preferably are obtained experimentally, but may be estimated from the particle-size distribution of the medium (e.g., Mishra, Parker, and Singhal 1989). Constitutive relations for three-phase flow used in MOFAT are scaled from the two-phase relations for water-NAPL and water-air and are predicated on the assumption that the relative wettability of solids is water > NAPL > air. The basis for the scaling procedure appears to be largely empirical.

Transport equations, a combination of the continuity and mass flux equations, must be solved for each constituent (≤5) in each phase (p = water, oil, air):

$$\phi S_p \frac{\partial C_{\alpha p}}{\partial t} = \frac{\partial}{\partial x_i}\left[\phi S_p D_{\alpha p ij} \frac{\partial C_{\alpha p}}{\partial x_j}\right] - q_{pi}\frac{\partial C_{\alpha p}}{\partial x_i} + R_{\alpha p} - \left(\lambda_{\alpha p} + \frac{R_p}{\rho_p}\right) C_{\alpha p} \tag{44}$$

where

$C_{\alpha p}$ = constituent α concentration in phase p

$D_{\alpha p ij}$ = dispersion tensor $[L \cdot T^{-1}]$

$\lambda_{\alpha p}$ = first-order decay coefficient $[T^{-1}]$ for component α associated with phase p

The continuity equation for the solid phase is:

$$\frac{\partial C_{\alpha s}}{\partial t} = R_{\alpha s} - \lambda_{\alpha s} C_{\alpha p} \tag{45}$$

where $C_{\alpha s}$ is the concentration of the constituent α per bulk, porous medium volume. Dispersion includes both molecular diffusion and hydrodynamic dispersion. The tortuosity model of Millington and Quirk (1959) is adopted to describe molecular diffusion in porous media. Hydrodynamic dispersion is modeled as dependent on seepage velocity and dispersivity, which may be anisotropic (longitudinal and transverse) (e.g., Bear 1972). Decay is modeled as a first-order loss (or gain if $\lambda < 0$) and may be defined for constituents in each phase.

NAPL constituents partition into the aqueous (dissolution), air (volatilization), and solid (adsorption) phases. Local equilibrium partitioning can be expressed in terms of linear coefficients: Raoult's constant for oil-water, Henry's constant for water-air, and K_d for water-solid partitioning. MOFAT takes a phase-summed approach to solving the transport equations

when equilibrium partitioning is assumed; equations are recast in terms of a single phase, usually either water or oil. Nonequilibrium partitioning uses apparent partitioning coefficients. An iterative solution is required to solve the nonlinear dependence of the apparent partitioning coefficients on concentrations and mass transfer rates.

Phase densities and mass transfer rates are updated at the end of each time step. This time-lagged updating imposes the assumption that changes in oil-water mass transfer rates and phase properties (density and viscosity) have a negligible impact on flow at the temporal scale of the time step—a weakly back-coupled process—though significant changes may develop over the course of the simulation. Additional assumptions include the following:

a. Darcy's Law is applicable and extendable to multiphase flow.

b. Constitutive relation parameters for multiphase flow are constant temporally, i.e., are not affected by changes in phase compositions.

c. NAPL constituents do not interact, allowing the decoupling of transport equations.

Numerical methods

MOFAT is a Galerkin finite element model. Spatial derivatives in the flow equations (see Equation 43) are solved with an asymmetric upstream-weighting function (after Huyakorn and Nilkuha 1978). Linear basis functions are used to handle the other terms. The model region is tessellated using linear quadrilateral elements (rectangular), i.e., Δx (or Δr) and Δz may be nonuniform but are constant for each element column and row, respectively. Nonlinear integration in the flow analysis is solved with a Newton-Raphson method with an implicit saturation derivative formulation of the governing equations. Convergence criteria can be defined in terms of the maximal and/or relative change in fluid heads (all phases, all nodes).

An adaptive solution domain (ASD) method is employed to avoid solving flow equations for immobile phases (absent or $\leq$ residual saturation) at a particular node. With the ASD method, phase flow is updated only after the change in phase head or saturation exceeds a user-specified tolerance.

Transport equations are solved alternately with flow equations (weak backcoupling). Phase-summed, transport equations are solved successively (decoupled) for each constituent by the upstream-weighted, Galerkin FEM. Phase densities are updated at the end of each time step. The model is finite-difference in time. The user specifies a time weighting factor (θ), from a fully implicit scheme ($\theta = 1$) to $0.5 \leq \theta \leq 1.0$, where $\theta = 0.5$ is a Crank-Nichoson scheme.

Evaluation

MOFAT performance is evaluated by assessing its application to the three example problems described in the documentation and additional

benchmark scenarios. MOFAT is not readily amenable to simple aqueous phase only flow and transport problems; therefore, benchmark problems for which analytical solutions are available are not evaluated here.

Documentation examples

Katyal, Kaluarachchi, and Parker (1991) include three example problems in the MOFAT documentation to demonstrate the code's basic capabilities and the input file structure; these include (a) one-dimensional infiltration and dissolution of a two-component LNAPL; (b) two-dimensional infiltration of a two-component LNAPL in Cartesian coordinates; and (c) two-dimensional infiltration of tetrachloroethene (PCE, a DNAPL) in radial coordinates. Neither analytical solutions nor experimental data are available with which to evaluate MOFAT performance on these hypothetical scenarios.

Example 1: Two-component LNAPL flow and transport in a 1-D column. Spill of a toluene and o-xylene mixture (equal mass fractions) into a homogeneous, vertical column is simulated in three stages: (a) LNAPL infiltration under constant head for 10.6 min, (b) redistribution for 25 days, and (c) constant water flux infiltration for 100 days. The lower 50 cm of the 200-cm column is initially water saturated; a constant water head BC is imposed at the bottom nodes.

The simulations generally ran in a manner consistent with the documentation description; output matched the documentation results (see Figure 46a,b). However, if the water flush (Stage 3, Figure 46c) is extended, the simulation encounters spurious oscillations in constiutent concentrations by Day 80, which increase until nonconvergence by Day 300. The root causes of these problems is uncertain, but likely is related to the use of oil-based phase-summed transport formulations in a system where one of the constituents becomes low due to simulated leaching (see Figure 47).

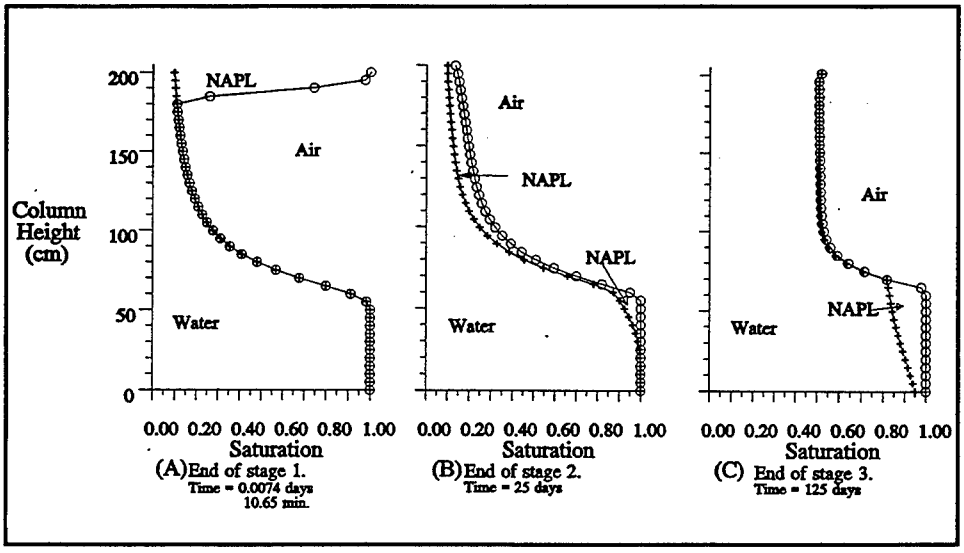

Figure 46. Saturation profiles for water (+) and total liquid (o) saturations at end of three stages

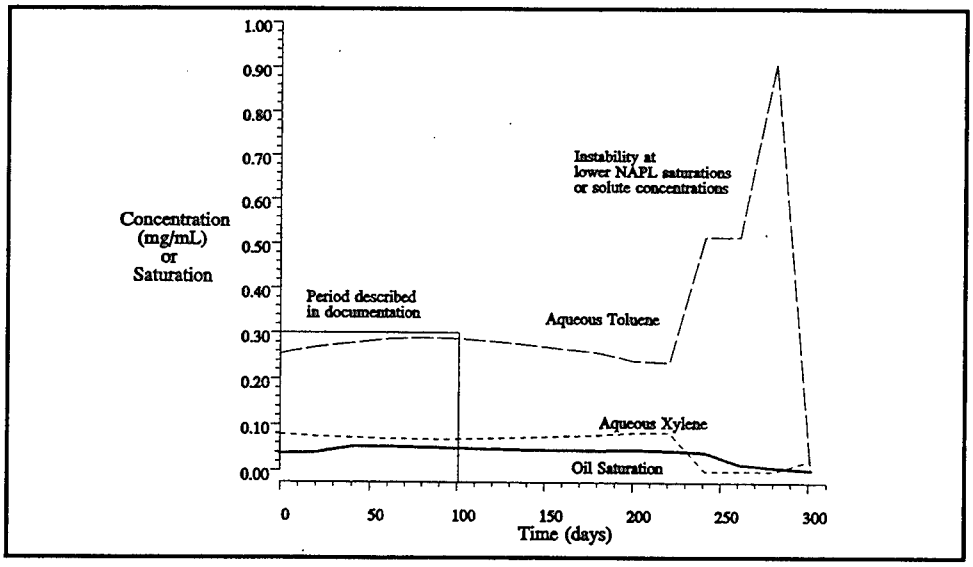

Figure 47. Effluent trends at Node 1 (bottom of column); simulation becomes unstable after 220 days

Example 2: 2-D spill of a two-component LNAPL in Cartesian coordinates. The release of 1 m^3 of a benzene (10.5 percent mass) and "inert oil" (89.5 percent) into a homogeneous 2-D field is simulated in two stages: (a) LNAPL infiltration under constant oil head for 4.17 days without solute transport, and (b) LNAPL redistribution for 25 days with transport simulated. A net water table gradient of 0.045 is maintained by the constant head boundary conditions imposed on the left and right sides.

Simulations matched the documentation results (Figures 48 and 49). However, if the redistribution stage is extended to allow the oil mass to further encounter the water table, numerical instabilities are evident after 45 days (see Figure 50). This instability may be due to problems encountered solving the strongly nonlinear flow equations. Smaller time steps may help.

Example 3: 2-D spill of a DNAPL (PCE) in radial coordinates. The release and vapor extraction of the DNAPL tetrachloroethene (a.k.a., perchloroethylene, PCE) into a homogeneous medium is simulated in radial coordinates with three stages: (a) infiltration from a surface source under constant NAPL head for 6.38 days (approximately 3 m^3), (b) DNAPL redistribution for 25 days with penetration through the saturated thickness, and (c) vapor extraction via a 2.5-m screened interval at constant air pressure head (h_a = -1.5 m). Results matched the documentation simulations (Figure 51).

None of the documentation examples demonstrate the utility of the ASD method. No guidance to appropriate levels of tolerance parameters are offered. Katyal and Parker (1992) describe application of ASD within MOTRANS, which involves more parameters than for MOFAT. Attempts to apply the ASD technique indicated that application is not straightforward. Applying the scale of ASD parameters utilized in Katyal and Parker (1992) to some of the documentation examples apparently induced nonconvergence or oscillations earlier than if ASD had not been used.

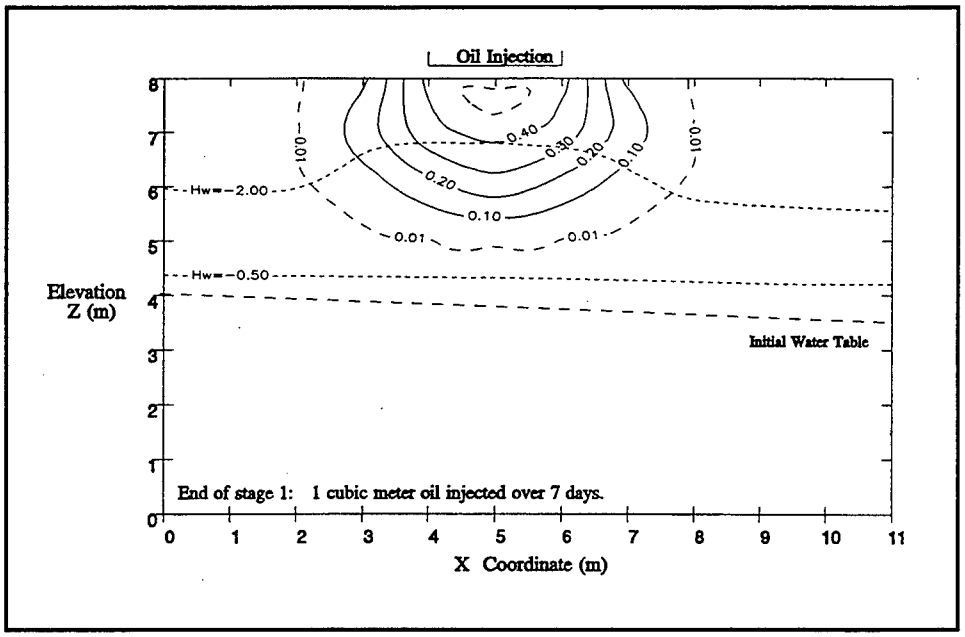

Figure 48. Oil saturation profile at end of Stage 1 (injection of 1 m^3 of LNAPL)

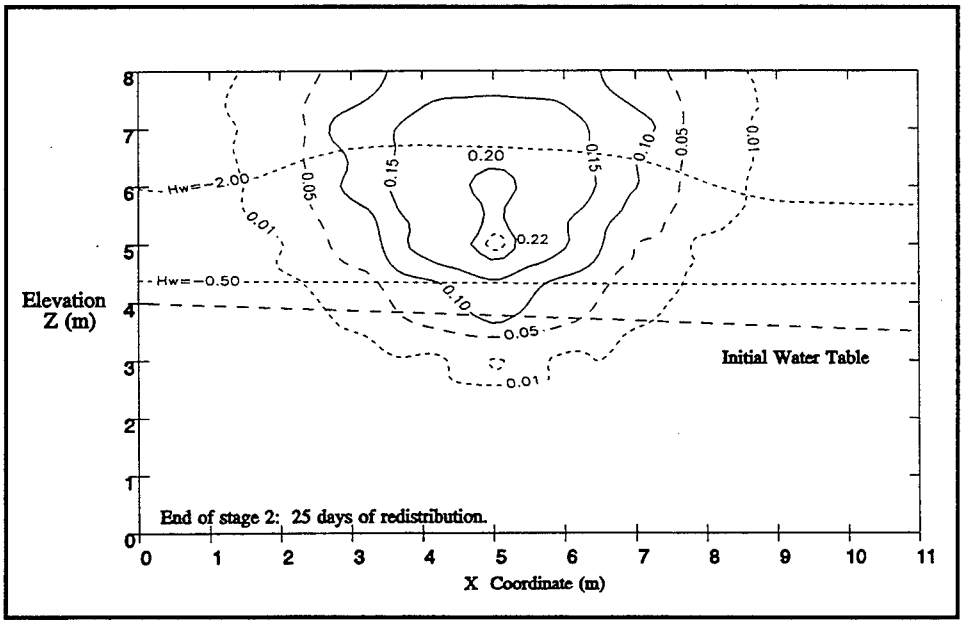

Figure 49. Oil saturation profile after 25 days of redistribution (end of Stage 2)

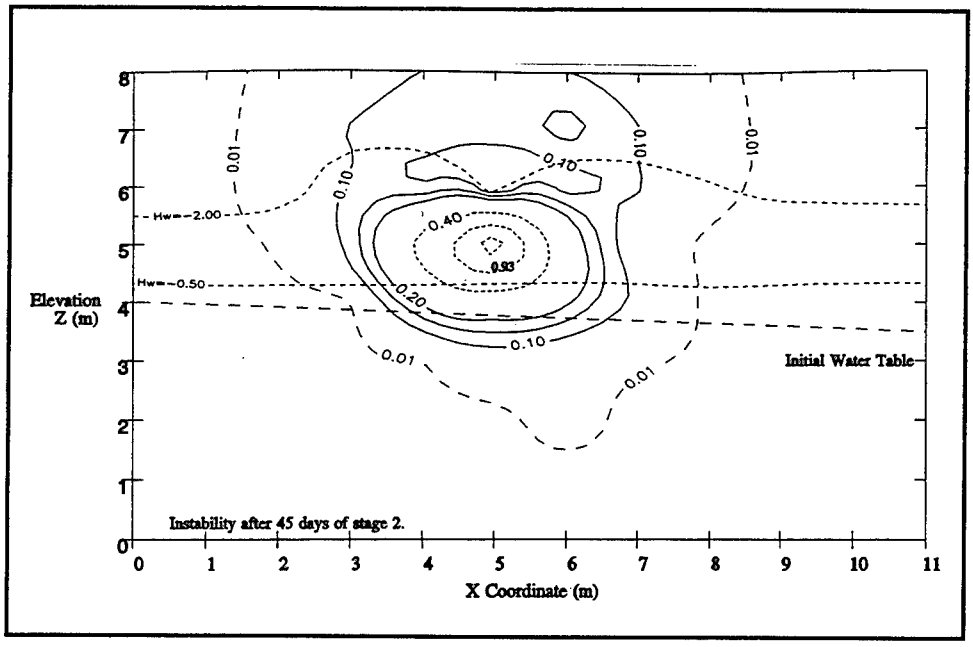

Figure 50. Oil saturation profile after 45 days of redistribution (numerical instability is evident by high erroneous saturation at center)

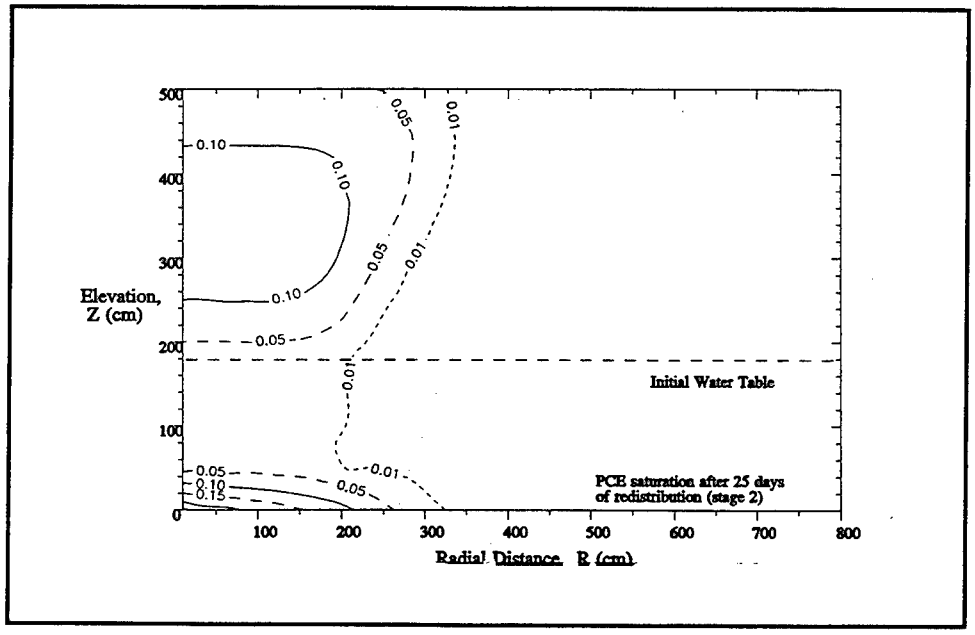

Figure 51. Oil saturation profile after 25 days of redistribution (end of Stage 2, Example 3)

Synthetic benchmarks

Thorough and reliable experimental data are rare for multiphase flow and transport problems. Until high quality data sets become available for model testing, an alternative approach is to define benchmark problems that will be encountered in the field.

Synthetic benchmarks for MOFAT and other multiphase codes are under development. For example, one benchmark under development is introducing a dense nonaqueous phase liquid (DNAPL) into a saturated-unsaturated, heterogeneous, stratified medium. Other public domain codes for multiphase flow and transport are being sought for comparative purposes.

One inevitable problem encountered in the field application of any contaminant transport or remediation code is how robust the model is in capturing the impacts of heterogeneous flow and transport properties. Natural permeability contrasts between adjacent sedimentary layers can be extreme (2 to 5 orders of magnitude). Even mildly heterogeneous media can be problematic for flow problems with highly nonlinear equations.

Heterogeneous media

A simple DNAPL release scenario into mildly heterogeneous is defined here for testing MOFAT. A small volume (0.5 m^3) of the PCE is released into a variably saturated medium with three material types—two discontinuous lenses, one of slightly lower permeability (K2 = K_z = 6 m/day; α = 4.99/m) and the other slightly more permeable (K3 = K_z = 8 m/day; α = 5.01/m), both within a sandy material (K1 = K_z = 7 m/day; α = 5.0/m; see Figures 52-56). No experimental data were available; thus, the model parameters are considered reasonable estimates based on scattered reports and summary tables in the documentation. Two stages were defined, the first for the PCE release, the second for redistribution.

MOFAT does not appear to be robust in its ability to solve the flow equations in heterogeneous media. The magnitude of the media property contrasts in the example presented is minimal by necessity. Virtually any contrast in the VG parameters (α, n) caused numerical instability. Only small variation in K_z could be solved with MOFAT.

Summary

MOFAT is one of very few, if not the only, public domain codes for multiphase flow and transport. The source code is available at nominal cost from the U.S. EPA Center for Subsurface Modeling Support (CSMOS) (RSKERL, Ada, OK). The current state of the art in multiphase flow and transport (MPFT) modeling is still rather inadequate. Regardless of the relative sophistication of MOFAT, all such models are of limited utility for field-scale application. Difficulties in site-specific parameter identification and uncertainties regarding subsurface processes and the influence

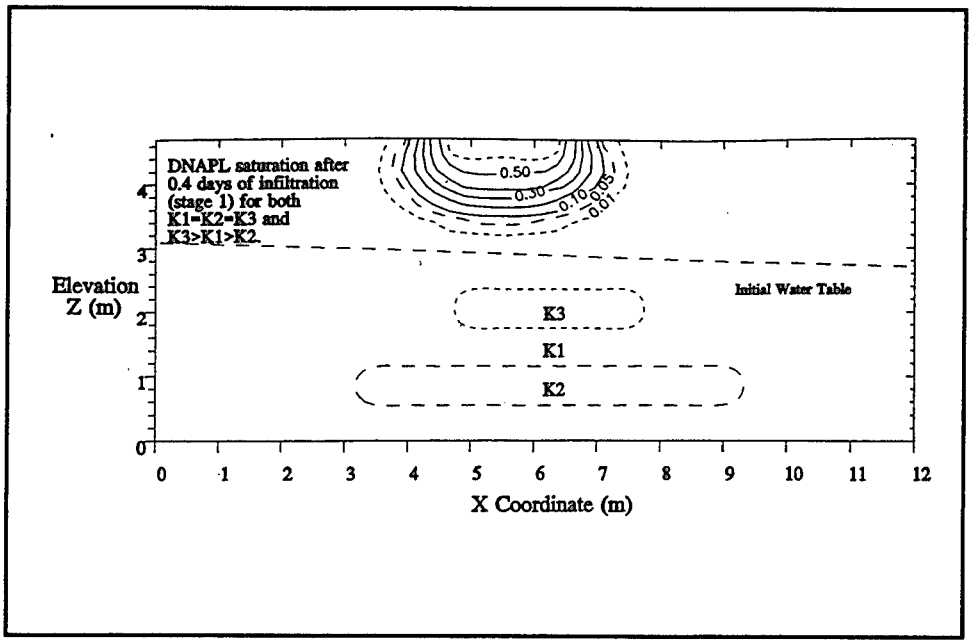

Figure 52. PCE liquid phase saturations after release of 0.5 m^3 over 7.5 hr (Same for both homogeneous and mildly heterogeneous media)

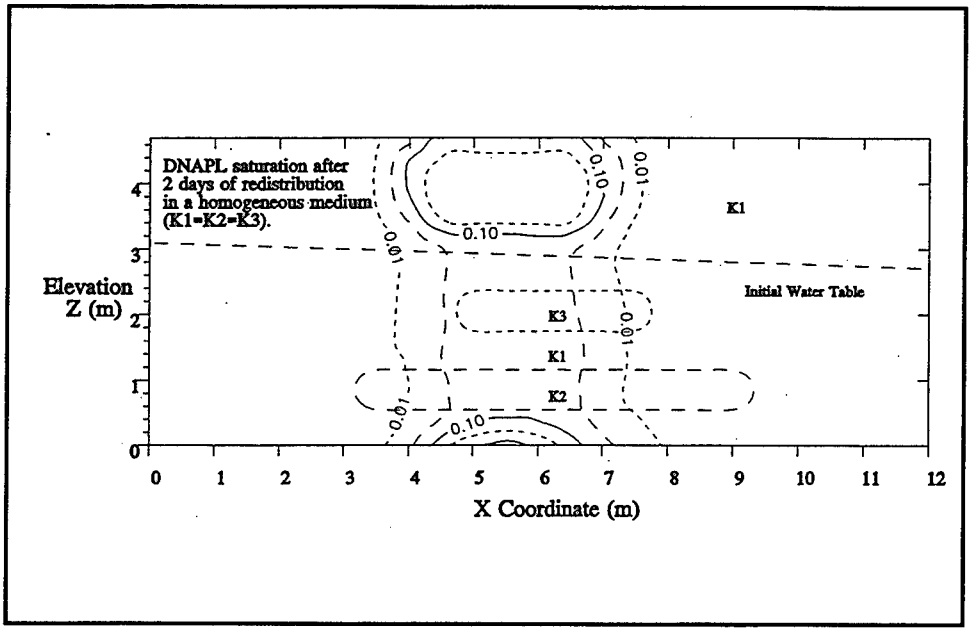

Figure 53. PCE liquid phase saturations after release of 2 days of redistribution in a homogeneous medium (K1 = K2 = K3)

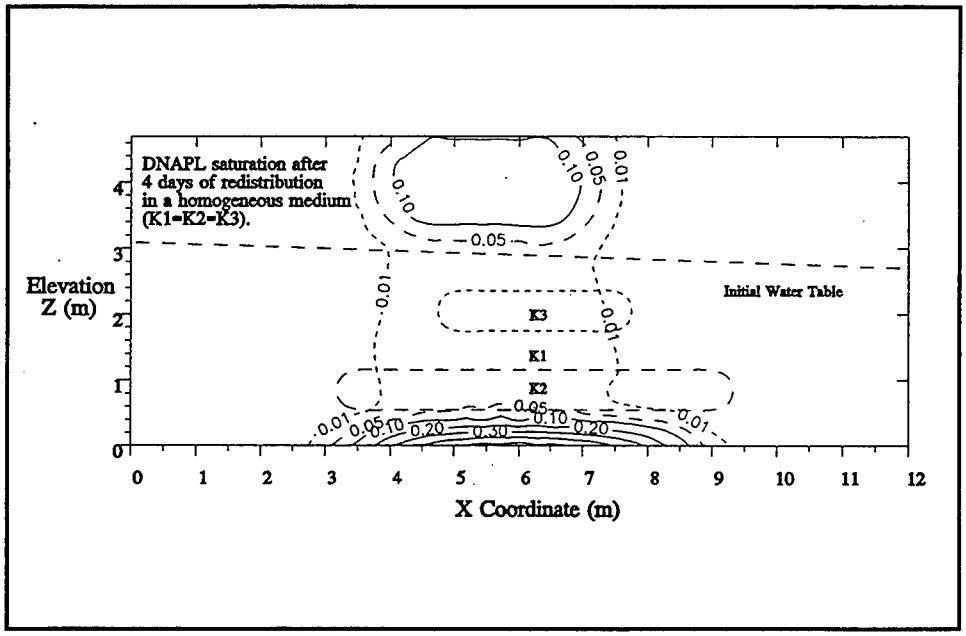

Figure 54. PCE liquid phase saturations after release of 4 days of redistribution in a homogeneous medium (K1 = K2 = K3)

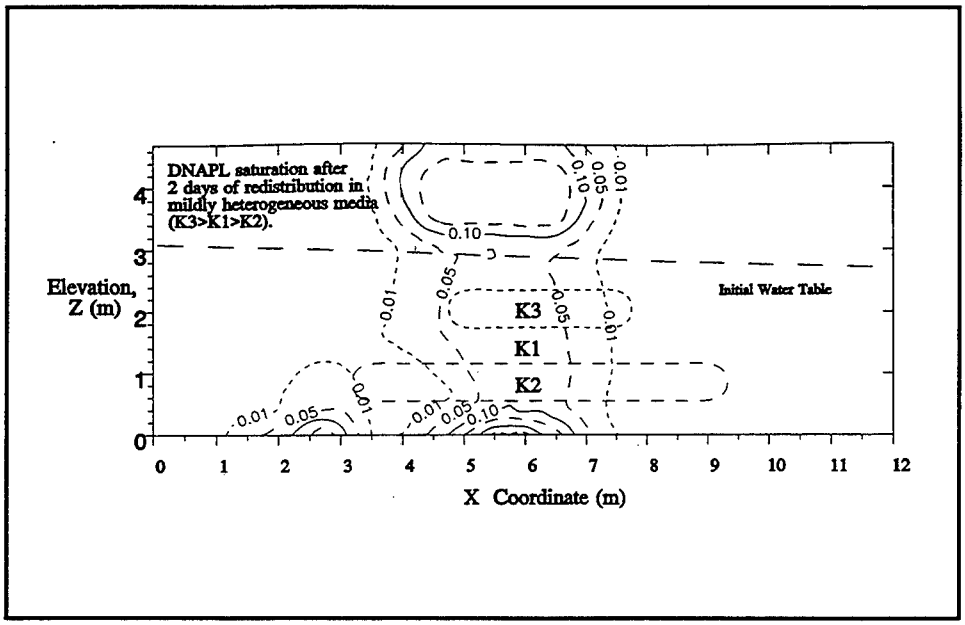

Figure 55. PCE liquid phase saturations after release of 2 days of redistribution in a mildly heterogeneous medium (K3 > K1 > K2)

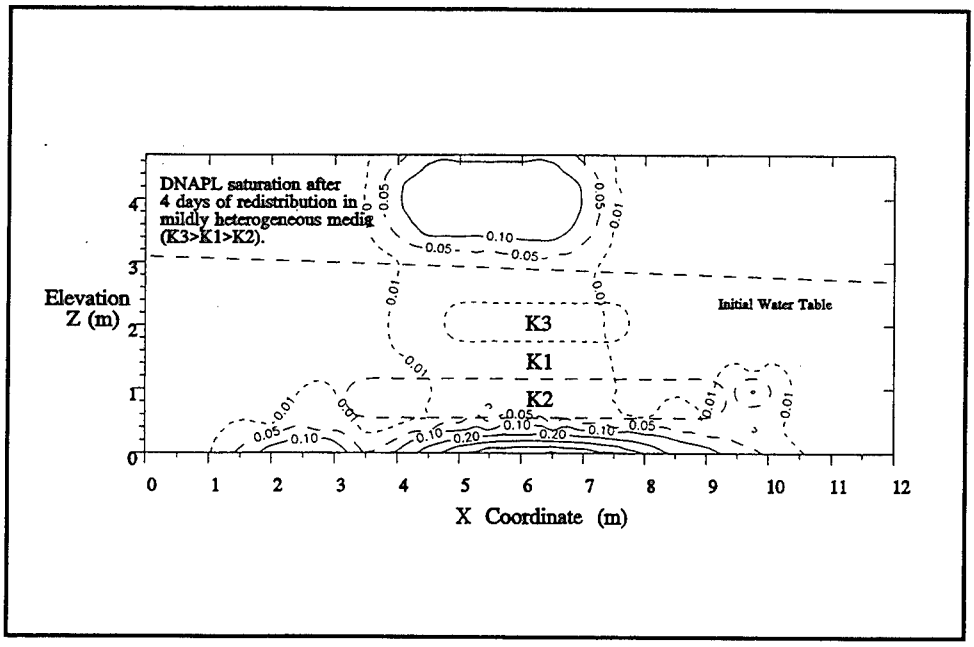

Figure 56. PCE liquid phase saturations after release of 4 days of redistribution in a mildly heterogeneous medium (K3 > K1 > K2)

of media heterogeneities relegate the current generation of codes to idealized process design.

Limited technical support for MOFAT is available from CSMOS. Environmental Systems and Technologies, Inc., developed MOFAT for the EPA and provides support for both MOFAT and MOTRANS.

Some of the limitations that impede the application of MOFAT, as well as other MPFT codes, to complex field simulations include the following:

- The MOFAT is a relatively new code (released in 1992) and therefore has a minimal track record for field applications. Likewise, MOTRANS (circa 1991) has had limited field application.

- Parameters for MPFT codes may be difficult to obtain, particularly the constitutive relation parameters. However, MOFAT is not unique in this regard. Any MPFT model likely would have the same problem.

Some specific limitations of MOFAT include the following:

- The assumption of noninteracting constituents in MOFAT, i.e., the partitioning of one does not affect the partitioning of another, is an acceptable assumption for mixtures of nonpolar, saturated hydrocarbons that are sparingly soluble in water. However, this assumption would fail for systems involving contaminants with polar functional groups (e.g., nitroaromatics, alcohols, phenols).

- The weak coupling between flow and transport assumed in MOFAT precludes application to remediation simulations involving strongly coupled processes, such as cosolvent flushing.

- Restriction to linear rectangular elements simplifies tessellation and supports use of the influence coefficient method, but defeats one of the major, potential advantages of the finite element method—the flexibility in adjusting the grid design to accommodate special features (wells, interfaces, etc.) or fitting irregular boundaries so common in the subsurface.

- Users cannot readily assign oil saturations as initial conditions, which one might want to do if residual saturation is assumed or saturations are known. One can assign the appropriate oil phase pressure based on the constitutive model.

- Several code features are not fully explained in the documentation; for example, the adaptive solution domain approach is described but never used in an example problem.

5 Model Evaluation Summary

MOC

MOC recommendations are based on both the evaluation results and the literature. Overall MOC performed satisfactory when evaluated. Figure 57 shows MOC developers and features. MOC evaluation highlights are as follows:

- USGS-MOC is a popular and well-established code that is well suited to the design of simple containment or remediation schemes (e.g., a screening model or pump-and-treat).
- The method of characteristics remains a useful tool for the simulation of advection-dominated transport.
- Lack of flexibility in discretization and boundary conditions limits the general applicability of USGS-MOC for remediation design. Other MOC-based transport codes offer greater flexibility and further development (e.g., MT3D with MODFLOW).

USGS-MOC is a mature code in that it is well documented and relatively "bug" free. Any problems are likely due to intrinsic limitations of the numerical methods or model design. The code can be obtained free of charge from the USGS through either bulletin boards or the Internet. If a hard copy manual is desired, then the code may be obtained from WATSTORE for a nominal charge. Due to its longevity and ease of use, the code is available through numerous vendors, including the following:

- U.S. Geological Survey WATSTORE; Reston, VA.
- Geraghty and Miller, Modeling Group; Reston, VA.
- International Groundwater Modeling Center, Golden, CO.
- Scientific Software Group, Washington, DC.

USGS - MOC (USGS - 2-D - TRANSPORT)	
Version	3.0 (11/89); MOC^{386}
Vendor (for the version tested herein)	Geraghty and Miller, Inc. 10700 Parkridge Boulevard, Suite 600 Reston, VA 22091 (703) 758-1200
Cost	$300 includes a utility to convert output files to SURFER grid files and extended memory version of the code. Cost varies among the vendors.
Developers	L. F. Konikow and J. D. Bredehoeft (1978) D. J. Goode and L. F. Konikow (1989) U.S. Geological Survey–Water Resources Division Reston, VA
Source Code	FORTRAN IV Public domain; available as document and ASCII file
Documentation	Adequate; USGS documents
Input/Output	User-designated input and output ASCII files Originally formatted input; input to support subsequent modifications are unformatted
Platform Platform Evaluated	PC to mainframe, depending on scale and complexity of the problem. The MOC^{386} version requires a 386 CPU, a math coprocessor, at least 1 MB of extended memory, and DOS 3.x. Evaluated on 486/33MHz machine with 8 MB RAM.
GMS Status	Not in the GMS

Figure 57. MOC highlights

MODFLOW

Figure 58 shows a summary of MODFLOW features. Because the MODFLOW model is very popular and is in the public domain, many vendors add some additional capabilities to the model and resell it.

The USGS still distributes the code in its basic form. Figure 59 lists some (not all) of the vendors that sell the MODFLOW program.

MODFLOW is recommended for groundwater flow problems that do not involve temperature variation, density variation (e.g., salt water and fresh water), unsaturated flow, or nonaqueous-phase contaminants. It is not applicable for fractures or heterogeneous porous media that cannot be reasonably represented by many, small rectangles.

For transport problems, MODFLOW can be used with a transport model such as MODPATH for advection only. Pathline codes, like MODPATH and GWPATH, that track the advective movement of a conservative tracer in the absence of dispersion are useful for preliminary analyses of

MODFLOW: A Modular Three-Dimensional Finite-Difference Groundwater Flow Model	
Version	MODFLOW PC/EXT v.1.31 (3/93)
Vendor (for the version tested herein)	International Ground Water Modeling Center (IGWMC) Colorado School of Mines Golden, CO 80401-1887 (303) 273-3103
Cost	$350 includes PREMOD, POSTMOD, and extended and virtual memory versions of the code. Cost varies among vendors. See the table of vendors later in this document.
Developers	Michael G. McDonald and Arlen W. Harbaugh (1984, 1988) U.S. Geological Survey, Reston, VA.
Source Code	Written in FORTRAN 66, minimally upgraded to FORTRAN 77. Code is in the public domain; source code is distributed.
Documentation	Adequate; USGS Reports
Input/Output	Input is from several ASCII files. Output consists of both formatted and unformatted files.
Platform	Designed to be portable and has been run on a variety of computer platforms. The executable program provided was compiled with Lahey's F77L-EM/32 v. 5.0 extended memory FORTRAN compiler. Execution requires an 80386/80486 processor with a math coprocessor, at least 2 MB of RAM, and at least 3 MB of hard disk space (more is recommended). With less than 4 MB of RAM, the virtual memory version of the model must be run, which is much slower.
Platform Evaluated	These evaluations were performed on an 80486/50MHz computer with 8 MB RAM.
GM Status	In the GMS

Figure 58. MODFLOW highlights

minimum travel times, contaminant origination, and for chasing problems in flow solutions. However, for quantitative evaluation of contaminant concentrations, a model like MT3D is needed. The MT3D program provides a much more realistic and detailed picture of transport than do advection-only pathline programs. The MT3D-compatible version of the model, MODFLOW/mt is probably a wise choice for use with MT3D because the linkages between the codes have already been performed.

Because of MODFLOW's popularity, many additional software routines and products are available to improve the usability or extend the capabilities of the MODFLOW program. Some were written by the USGS and others by private companies. Table 8, although quite long, is an incomplete list of the many products available.

Some Vendors of the MODFLOW Program			
Model Name	**Distributor**	**Cost**	**Includes**
MODFLOW	USGS	$40	Support by the USGS.
MODFLOW PC-EXT	International Ground Water Modeling Center	$350	Extended and virtual memory versions with PREMOD and POSTMOD.
MODFLOW^{EM}	Scientific Software Group	$339	Extended memory version includes ZONEBUDGET and technical support from McDonald-Morrisey Associates.
MODFLOW^{386}	Geraghty and Miller	$300	Extended memory version with utilities and support.
MODFLOW^{MAC}	Geraghty and Miller	$375	Macintosh version of the MODFLOW program. Includes support.
MODFLOW/mt	S. S. Papadopulos and Associates, Inc.	Included with MT3D	Extended memory version with utilities. Writes the unformatted file containing data required by MT3D.
MODFLOWP	USGS	$40	Basic program plus parameter estimation capability.

Figure 59. MODFLOW vendors (Not a complete listing but is intended to provide an example. Inclusion herein does not indicate sanction by the U.S. Government, etc.)

Table 8
Support Software for MODFLOW

Program Title	Developer (if known)	Distributor (addresses below)	Cost	Brief Description
RADMOD	Riley and Harbaugh	USGS	$40	Computes cylindrical flow to a well.
MODMAN	Greenwald	GeoTrans, Inc.	$1,500	Optimization of pumping rates in MODFLOW.
ZONEBUDGET	Harbaugh	USGS	$40	Calculates subregional water budgets such as flow to/from a river, etc.
MODINP	TECSOFT, Inc.	Scientific Software Group	$150	Preprocessor for MODFLOW input files.
MODELCAD^{386}	Rumbaugh	Geraghty and Miller	$750	Graphical preprocessor for MODFLOW, MOC, MT3D, and MODPATH.
MMSP	Scott	USGS	$40	Statistical processor for analyzing MODFLOW output.
PM	Chiang and Kinzelbach	Scientific Software Group	$350	Graphical preprocessor and postprocessor for MODFLOW and MODPATH.

(Continued)

Table 8. (Concluded)

Program Title	Developer (if known)	Distributor (addresses below)	Cost	Brief Description
MODFLOW[386] Utilities		Geraghty and Miller	$100	Includes conversion programs for unformatted to ASCII, and for SURFER graphics, also calibration statistics, etc
MODPATH	David Pollack	USGS	$40	Particle tracking for steady-state, advection-only transport.
MODPATH[EM]	David Pollack	Scientific Software Group	$350	Extended memory version of the USGS model. Supported.
MODPATH-PLOT[EM]	David Pollack	USGS	$350	Display/analysis of MODPATH results. Supported.
MODGRAF[EM]		Scientific Software Group	$425	Creates velocity vectors and head contour plots from MODFLOW output.
MODINV[EM]		Scientific Software Group	$800	Modeling tool kit including MODFLOW, parameter estimation, and preprocessor and postprocessors.
MODVEL[EM]		Scientific Software Group	$150	Creates an unformatted velocity file for use by MODGRAF.
MODCELL[EM]		Scientific Software Group	$150	Converts unformatted cell-by-cell flow terms to ASCII files for viewing/printing.
MODLOCAL[EM]		Scientific Software Group	$995	Constructs local MODFLOW input files from regional MODFLOW files.
MODRET		Scientific Software Group	$325	Couples MODFLOW with an infiltration program to simulate storm water retention ponds.
MPATHIN[EM]	TECSOFT, Inc.	Scientific Software Group	$150	Preprocessor for MODPATH.
SURFER		Golden Software, Inc.	$499	Graphics program for displaying contours and surface maps.

MT3D

For a saturated medium in which the flow and transport solutions can be decoupled, the use of MODFLOW/mt with MT3D is recommended. The models are sufficiently simple that set up, and modification can be performed in a reasonable time frame. However, when combined, these models have most capabilities required for routine saturated-zone flow and transport modeling.

Although users new to MT3D and MODFLOW likely will be overwhelmed with the abundance of input possibilities and choices for output formats and locations, those already familiar with MODFLOW will be immediately comfortable with MT3D's structured, uncommented style of ASCII input files. The program was constructed to be an add-on to MODFLOW, although it will accept head information from other sources.

There are many advantages to this linkage. The MODFLOW package is very dynamic with a large user community that is developing additional modules or packages to solve previously unresolved problems.

Overall, if the user can live with some of the mass balance "errors" that the MOC solution inherently carries, and the limitations of MODFLOW as discussed previously, then the MODFLOW/mt with MT3D package is recommended. Figure 60 shows MT3D features.

MODFLOW is already included in the Groundwater Modeling System (GMS), the WES-developed comprehensive graphical environment for numerical modeling. The GMS provides tools for site characterization, model conceptualization, mesh and grid generation, geostatistics, and post-processing. MT3D was included in the GMS by the end of FY95.

MT3D: A Modular Three-Dimensional Transport Model	
Version	1.8 (10/92)
Vendor/Distributor	S. S. Papadopulos and Associates, Inc. (SSP&A) 7944 Wisconsin Avenue Bethesda, MD 20814 (301) 718-8900 Center for Subsurface Modeling Support (CSMoS) (Version 1.2 only) Robert S. Kerr Environmental Research Laboratory USEPA P.O. Box 1198 Ada, OK 74820 (405)436-8500
Cost	$450 including MT3D source code and executable, utility programs, and MODFLOW/mt (SSP&A's MODFLOW)
Developer	Chunmiao Zheng (1990, 1992, 1993), formerly at SSP&A, now at the University of Alabama
Source Code	FORTRAN 77 (except the IMPLICIT NONE statement). The executable provided contains FORTRAN 90 dynamic memory allocation. Proprietary program but source code is distributed.
Documentation	Very Good
Input/Output	Input from the flow solution is unformatted. Most other input and output files are ASCII files.
Platform Platform Evaluated	PC to mainframe, depending on complexity of problem. The executable program provided was compiled with Lahey's F77L-EM/32 v. 5.01 extended memory FORTRAN compiler. Execution requires an 80386/80486 processor with math coprocessor, at least 2 MB of RAM and at least 1 MB of hard disk space (more is recommended). These evaluations were performed on an 80486/50MHz computer with 8 MB RAM
GMS Status	Was included in the GMS by late FY95

Figure 60. MT3D highlights

PLASM

PLASM is an excellent teaching tool, has significant support, and is recommended as a screening model. PLASM runs on many platforms, is efficient, and has significant third-party support. PLASM needs a graphical interface to facilitate its use as a screening model. Figure 61 presents a summary of PLASM's features.

PLASM	
Version	2.0 (8/90); IGWMC # FOS12
Vendor/Distributor	International Ground Water Modeling Center (IGWMC) Colorado School of Mines Golden, CO 80401-1887 (303) 273-3103
Cost	$120 includes a package of three finite-difference programs and a preprocessor.
Developer	T. A. Prickett and C. G. Lonquist Illinois State Water Survey Champaign, IL 1971
Language	FORTRAN 77.
Code	Complete source code, documentation, example input data sets, and executables (CONPLASM, UNCPLASM, and PREPLASM) provided on floppy disks.
Documentation	Documentation includes that describing the modifications by Paul van Der Heijde and the original Illinois State Water Survey Bulletin 55.
Input	Input data files were created using the preprocessor PREPLASM. Once the input data file is created with PREPLASM, then the file is copied into either conplasm.i05 or uncplasm.i05 file and the PLASM program is executed.
Output	Output files created by PLASM (CONPLASM or UNCPLASM) are plasm.o06 and plasm.o08. The file plasm.o06 is an echo of the input data; the file plasm.o08 is the head distribution for the simulation.
Platform Platform Evaluated	PC to mainframe, depending on the scale and complexity of the problem. The IGWMC version is compiled with Microsoft FORTRAN Version 4.1, and the preprocessor was compiled with QuickBasic 4.0. Minimum hardware requirements are a PC-compatible 8086/80286/80386/80486 based system with 640 K RAM and DOS 2.0 or higher. Evaluated on a 486/66MHz PC with 32 MB of RAM.
GMS Status	Not in the GMS

Figure 61. PLASM's features

RANDOM WALK

RANDOM WALK and RAND3D are the two- and three-dimensional groundwater models for solute transport based on the RANDOM-WALK algorithm. Both models have a significant number of users in private consulting and in the Army. RAND3D is fairly easy to use once a user becomes familiar with the code. A graphical user interface will significantly benefit both models, since input file generation is painful. Most of the concerns associated with RAND3D should be resolved with its new release. Figures 62 and 63 summarize both RANDOM WALK and RAND3D, respectively.

RANDOM WALK	
Version	1.0; IGWMC FOS # 13
Vendor/Distributor	International Ground Water Modeling Center (IGWMC) Colorado School of Mines Golden, CO 80401-1887 (303) 273-3103
Cost	$100 includes FORTRAN source, executable, and three example data sets for the IGWMC RANDOM WALK.
Developer	T. A. Prickett, T. G. Naymik, and C. G. Lonnquist Illinois State Water Survey Champaign, IL 1981
Language	FORTRAN 77.
Code	Complete source code, executable, and three example data sets provided on floppy disk.
Documentation	Complete, includes two Illinois State Water Survey reports: Bulletins 55 and 65.
Input	Example problems available on floppy disk.
Output	Output files that can be displayed on SURFER.
Platform Platform Evaluated	486 PC to mainframe, the version evaluated was for the PC-compatible environment: 80286/80386/80486. Minimum requirements are 640 KB of RAM and a minimum of 1 MB of disk space, although more is recommended. Evaluated on a 486/25MHz PC with MB of RAM.
GMS Status	Not in the GMS

Figure 62. RANDOM WALK highlights

RANDOM WALK-3D	
Version	RAND3D
Vendor/Distributor	RANDOM WALK-3D Donald Koch Engineering Technologies Associates 3458 Ellicott Center Drive Ellicott City, MD 21043 (301) 461-9920
Cost	No charge, includes basic source code, executable, an example data set, and PREMOD3D (a preprocessor that creates input files for RAND3D from MODFLOW output.
Developer	Donald Koch (Same as distributor)
Language	Microsoft Quick Basic
Code	Basic source code provided on a floppy disk; the preprocessor PREMOD3D is written in FORTRAN. Code is interactive.
Documentation	Available.
Input	Data file (head) from a groundwater flow model like MODFLOW. Example problem is included with the model on floppy disk.
Output	Results are displayed graphically.
Platform Platform Evaluated	PC only. Execution requires an 80286/80386/80486 processor with math coprocessor, at least 640 KB of RAM, and at least 1 MB of hard disk space (more is highly recommended). Evaluated on a 486MHz PC.
GMS Status	Will be included in the GMS in late FY97 or early FY98.

Figure 63. RAND3D highlights

FEMWATER and LEWASTE

The models did an acceptable job of simulating the unsaturated/ saturated flow in porous media tested. The models have a significant number of choices and options; with the aid of a graphical user interface, FEMWATER/LEWASTE should be considered for many subsurface problems. Figures 64 and 65 describe the most important features, vendors, and developer of both models. Both models are now part of the GMS.

FEMWATER	
Version	3-D EPA.
Vendor/Distributor	Same as developer, Dr. George Yeh
Cost	N/C
Developer	G. T. (George) Yeh Department of Civil Engineering Pennsylvania State University University Park, PA 16802
Language	FORTRAN 77.
Code	Complete source code provided in an ASCII file on floppy disk.
Documentation	Complete report in WordPerfect 5.1 format on floppy disk.
Input	Data file partly in fixed and partly in free-field format. Example problems available on floppy disk.
Output	Results are placed in files. Only information for selected time steps are output.
Memory Requirements	Vary depending on size of problem. Easily adjustable by changing PARAMETER statements in .inc files.
Platform Platform Evaluated	486 PC or Unix workstation for small problems. Supercomputer for large problems. Silicon Graphics workstation
GMS Status	In the GMS

Figure 64. FEMWATER characteristics

LEWASTE	
Version	3-D EPA.
Vendor/Distributor	Same as developer, Dr. George Yeh
Cost	No charge
Developer	G. T. (George) Yeh Department of Civil Engineering Pennsylvania State University University Park, PA 16802
Language	FORTRAN 77.
Code	Complete source code provided in an ASCII file on floppy disk.
Documentation	Complete report in WordPerfect 5.1 format on floppy disk.
Input	Data file partly in fixed and partly in free-field format. Example problems available on floppy disk.
Output	Results are placed in files. Only information for selected time steps are output.
Memory Requirements	Vary depending on size of problem. Easily adjustable by changing PARAMETER statements in .inc files.
Platform Platform Evaluated	486 PC or Unix workstation for small problems. Supercomputer for large problems. Silicon Graphics workstation.
GMS Status	In the GMS.

Figure 65. LEWASTE characteristics

UNSAT1

UNSAT1 simulates flow in the unsaturated or vadose zone. The model's performance was similar to that of CHEMFLO; thus it is recommended that a program like CHEMFLO or PRZM-2 be included for further evaluation rather than UNSAT1. Both CHEMFLO and PRZM-2 include solute transport which UNSAT1 lacks. Figure 66 summarizes UNSAT1.

UNSAT1: A One-Dimensional Finite Element Model for Unsaturated Flow	
Version	1.0; IGWMC-FOS 18 PC
Vendor (for the version tested herein)	International Ground Water Modeling Center (IGWMC) Colorado School of Mines Golden, CO 80401-1887 (303) 273-3103
Cost	$50 includes PREMOD, POSTMOD, and extended and virtual memory versions of the code. Cost varies among vendors. See the table of vendors later in this document.
Developers	M. Th. van Genuchten Princeton University, Princeton, NJ
Source Code	Written in ANSI FORTRAN. Code is in the public domain, source code is distributed.
Documentation	Adequate, USGS Reports
Input/Output	Input is from several ASCII files. Output consists of both formatted and unformatted files.
Platform	Variations/modifications of UNSAT1 may be run on different platforms. The executable program provided was compiled with Microsoft's FORTRAN Version 3.2 compiler. Execution requires an IBM-PC, XT, AT, 80386/80486 processor with a math coprocessor, at least 512 K of RAM, and DOS 2.0 or above.
Platform Evaluated	These evaluations were performed on an 80486/66MHz computer with 8 MB RAM.
GMS Status	Not in the GMS

Figure 66. UNSAT1 highlights

CHEMFLO

CHEMFLO performed satisfactorily in the unsaturated zone evaluation. The software is a good screening tool and an excellent teaching tool. The model/software is recommended for simple unsaturated zone flow and transport modeling. In addition, it is highly recommended as a "first cut" approach, especially for unsaturated zone problems lacking soil and chemical data.

CHEMFLO compares favorably with UNSAT1, another one-dimensional unsaturated flow model, in simulating Prill, Johnson, and Morris's (1965) column drainage experiment. One advantage that CHEMFLO has over UNSAT1 is its "user friendly" interface. Figure 67 highlights CHEMFLO's features.

CHEMFLO: A One-Dimensional Water and Chemical Transport Model	
Version	1.3
Vendor/Distributor	Center for Subsurface Modeling Support (CSMoS) Robert S. Kerr Environmental Research Laboratory USEPA P.O. Box 1198 Ada, OK 74820 (405) 436-8500
Cost	No charge for executable and example case.
Developer	D. L. Nofziger, K. Rajender, Sivaram K. Nayudu, and Pei-Yao Su (1989) Department of Agronomy Oklahoma State University Stillwater, OK
Source Code	None
Documentation	Good; EPA manual.
Input/Output	Interactive input. There is a soils properties database file included with the executable. Output files are ASCII files.
Platform	PC only. Execution requires an 80286/80386/80486 processor with math coprocessor, at least 640 KB of RAM, and at least 1 MB of hard disk space (more is highly recommended).
Platform Evaluated	These evaluations were performed on an 80486/66MHz computer with 32 MB RAM.
GMS Status	Not in the GMS

Figure 67. CHEMFLO characteristics

PRZM-2

PRZM-2 is a collection of models to predict pesticide fate and transport in agricultural soils. The tool consists of two modules: PRZM, a pesticide root zone model, and VADOFT, a vadose zone model. The model has an extensive chemical database, has guidance on parameter selection for different areas of the country, and incorporates meteorological inputs.

The model needs an interactive or graphical user interface. PRZM-2 would benefit significantly from a modeling system such as the GMS. Model evaluation up to this point consisted of examples included with the documentation. PRZM-2 will be evaluated with chemical field data in the near future. The model is highly recommended for sites where crops or plant growth is significant. Figure 68 shows PRZM-2's features.

PRZM-2: Pesticide Fate in the Crop Root and Unsaturated Soil Zones	
Version	1.02
Vendor/Distributor (for the version tested herein)	Center for Exposure Assessment Modeling (CEAM) Environmental Research Laboratory U.S. Environmental Protection Agency 960 College Station Road Athens, GA 30606-2720 (706) 546-3549
Cost	No charge; includes WordPerfect documentation and an extended memory version of the code.
Developers	J. A. Mullins, R. F. Carsel, J. E. Scarbrough, and A. M. Ivery (1993) AScI Corporation Athens, GA U.S. Environmental Protection Agency Athens, GA
Source Code	FORTRAN-77 Public domain; available as document and ASCII file
Documentation	Good; EPA manual
Input/Output	Several input files are needed for a PRZM2 run; as a minimum a meteorological file (MET.INP), a command file (PRZM2.RUN), and at least one of the modules files: PRZM.INP, VADOFT.INP, and/or MC.INP Output files consist of the run output file PRZM.OUT and the time series (TIMES.OUT and VADF.OUT) files from the PRZM module and the vadose module.
Platform Platform Evaluated	PC, PRIME 50 minicomputer, SUN SPARC under UNIX/SUNOS,and DEC VAX systems. The executable program provided was compiled with Lahey's F77-EM/32 version 5.01. Execution requires a 386 or 486 CPU, a math coprocessor, 640 K base memory, at least 4 MB of extended memory, at least 4.5 MB of hard disk space and DOS 3.x or higher. Evaluated on 486/66MHz machine with 8 MB RAM.
GMS Status	Not in the GMS

Figure 68. PRZM-2 overview

SUTRA

SUTRA performed favorably in overall evaluation, including the example evaluation, the test cases, and Vauclin's experiment. The model is very versatile and powerful, has a significant user group, and shows promise for future development. Figure 69 shows its highlights. SUTRA is available through numerous vendors, including the following:

- U.S. Geological Survey WATSTORE; Reston, VA.
- Geraghty and Miller, Modeling Group; Reston, VA.
- International Groundwater Modeling Center, Golden, CO.
- Scientific Software Group, Washington, DC.

SUTRA: Saturated-Unsaturated TRAnsport	
Version	SUTRA^{386} Version 1.0
Vendor (for the version tested herein)	Geraghty and Miller, Inc. 10700 Parkridge Boulevard, Suite 600 Reston, VA 22091 (703) 758-1200
Cost	$300 includes postprocessing utility to convert output files to SURFER grid files and extended and virtual memory versions of the code. Cost varies among vendors. See the table of vendors later in this document.
Developers	Clifford I. Voss (1984) WRIR 84-4369 U.S. Geological Survey, Reston, VA.
Source Code	Written in standard ANSI FORTRAN. Code is in the public domain.
Documentation	Adequate-good, USGS Reports
Input/Output	Input is from two ASCII files. One with all of the data necessary for simulation, the other with initial conditions of pressure and concentration or temperature. Output consists of one or two files. One contains the output of the simulation; the second is optional and contains output at a time step similar to the initial conditions. The second output file is used for restart.
Platform	The executable program provided was compiled with Lahey's F77L-EM/32 FORTRAN compiler and the OS/386 software developed by Ergo Computing, Inc. Execution requires an 80386/80486 processor with a math coprocessor, at least 1 MB of RAM. The executables included in the version evaluated required 1 MB, 3 MB, or 7 MB of RAM.
Platform Evaluated	These evaluations were performed on an 80486/66MHz computer with 32 MB RAM.
GMS Status	Not in the GMS

Figure 69. SUTRA highlights

VS2DT

VS2DT performed favorably for problems provided in its user's manual. In addition, the program was examined against a published laboratory experiment and numerical solution. Results of VS2DT simulations were in good agreement with the published data. The example problems involved physical processes such as infiltration, evaporation, evapotranspiration, and injection wells in radial flow. The soil conditions in these examples ranged from fully saturated, to fully unsaturated, to mixed unsaturated-saturated zone conditions. The fluid density in VS2DT is fixed to be 1.0 g/cm^3. Hence, all other parameters must be input in units of grams and centimeters; time can be in seconds, minutes, hours, etc.

VS2DT required small time steps and fine spatial discretization to achieve convergence and obtain a stable solution for the unsaturated-saturated example problem (Vauclin's Experiment). VS2DT has four options to specify the water-retention relationship between pressure head and water content. These options are a user-defined or measured value, the Brooks-Corey equation, the Haverkamp equation, and the van Genuchten formulation. All options were tested using the default parameters coded in VS2DT. The user-defined or tabulated option for pressure head-water content did not work properly.

Overall, VS2DT shows promise as a saturated and couple unsaturated/ saturated groundwater code. The code needs some modifications to make it more general and easier to use; there should be no need to recompile the code to select different options. The code would benefit from the GMS interface. Figure 70 shows VS2DT's characteristics, developer, and other relevant information. Refer to the list of vendors in the previous section for VS2DT resellers.

VS2DT: Solute Transport in Variably Saturated Porous Media 0	
Version	VS2DT386 Version 1.0
Vendor (for the version tested herein)	Geraghty and Miller, Inc. 10700 Parkridge Boulevard, Suite 600 Reston, VA 22091 (703) 758-1200
Cost	$300 includes postprocessing utility, extended and virtual memory versions of the code. Cost varies among vendors. See the table of vendors later in this document
Developers	R. W. Healy (1990) WRIR 90-4025 (Transport) E. G. Lappala, R. W. Healy, and E. P. Weeks (1987) WRIR 83-4099 (Flow) U.S. Geological Survey, Reston, VA.
Source Code	Written in standard ANSI FORTRAN. Code is in the public domain.
Documentation	Adequate, USGS Reports
Input/Output	Input is from several ASCII files. Output consists of both formatted and unformatted files.
Platform	The executable program provided was compiled with Lahey's F77L-EM/32 FORTRAN compiler and the OS/386 software developed by Ergo Computing, Inc. Execution requires an 80386/80486 processor with a math coprocessor, at least 1 MB of RAM.
Platform Evaluated	These evaluations were performed on an 80486/66MHz computer with 24 MB RAM.
GMS Status	Not in the GMS

Figure 70. VS2DT characteristics

MOFAT and MOTRANS

MOFAT results matched the documentation simulations well. The current state of the art in multiphase flow and transport (MPFT) modeling is still inadequate. Regardless of the relative sophistication of MOFAT, all such models are of unknown utility in field-scale application. Difficulties in site-specific parameter identification and uncertainties regarding subsurface processes and the influence of media heterogeneities relegate the current generation of codes to idealized process design.

MOFAT is presently the only readily available multiphase flow and transport code in the public domain. Other codes are either for multiphase flow only or assume residual NAPL saturation. Figure 71 shows MOFAT's features and distribution sources.

MOFAT's limitations as a remediation model are those expected of a fairly new and complex model. In particular, the code has a minimal track record for field applications; parameters for MPFT codes may be difficult to obtain, particularly the constitutive relation parameters; and MOFAT treats NAPL constituents as noninteracting, i.e., the partitioning of one does not affect the partitioning of another.

On the other hand, MOFAT is capable of simulating NAPL release, dispersal, and partitioning into aqueous and vapor phases. Predictions of free (mobile) and residual NAPL distribution are possible. The code is recommended for pump-and-treat and vapor extraction recovery systems where NAPL are present. Figure 72 presents a list of groundwater software vendors.

MOFAT	
Version	1.0 (1991)
Source/Vendor	Center for Subsurface Modeling Support (CSMoS) R. S. Kerr Environmental Research Laboratory (RSKERL) U.S. EPA - Office of Research and Development Ada, OK 74820 (405) 332-8800 (x245)
Developers	Kaluarachchi and Parker (1989, 1990) Katyal, Kaluarachchi, and Parker (1991) Center for Environmental and Hazardous Material Studies Virginia Polytechnic Institute and State University Blacksburg, VA 24061-0404
Source Code	FORTRAN 77 MOFAT: public domain, available as ASCII file from CSMoS MOTRANS: proprietary version; executables only from ES&T
Documentation	Document prepared for EPA-RSKERL
Input /Output	Formatted ASCII input files; PREMOF: menu-driven, preprocessor with MOFAT. Output files are formatted ASCII; user has some control over frequency of output
Platform Platform Evaluated	Dependent on scale and complexity of the simulation. MOFAT optimally requires 10 MB RAM on a 386-CPU with math coprocessor (or 486). MOFATVM is a virtual memory version with more reasonable RAM requirements, though at a speed cost. MOFATVM was evaluated on 486/33MHz machine with 8 MB RAM.
GMS Status	Not in the GMS

Figure 71. MOFAT highlights

Vendors' Addresses

USGS
Water Resources Division
437 National Center
12201 Sunrise Valley Drive
Reston, VA 22092
(703) 648-5695

Geraghty and Miller, Inc.
Modeling Group
10700 Parkridge Boulevard
Suite 600
Reston, VA 22091
(703) 758-1200

Golden Software, Inc.
809 14th Street
Golden, CO 80402-0281
(303) 279-1021

GeoTrans, Inc.
46050 Manekin Plaza
Suite 100
Sterling, VA 20166
(703) 444-7000

Scientific Software Group
P.O. Box 23041
Washington, DC
(703) 620-9214

S. S. Papadopulos and Associates, Inc.
7944 Wisconsin Avenue
Bethesda, MD 20814
(301) 718-8900

International Ground Water Modeling Center
Colorado School of Mines
Golden, CO 80401-1887
(303) 273-3103

Figure 72. General groundwater software vendors

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Appendix A: Abbreviated List of Subsurface Models

Table A1
Analytic Single-Phase Flow and Transport Models

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Time Solution	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Analytic Flow Solutions								
ANALYTICAL MODELS	Earthware of California	2-D	Time varying	Porous; confined/ unconfined/ semiconfined	None	Preprocessor and postprocessor, user's instructions, sample problems, supported; with graphics	Unknown	Up to 100 by 100 grid with 50 wells
BEAVERSOFT	Bear and Verruijt (1987) International Ground Water Modeling Center (IGWMC)	1-D and 2-D	Unknown	Varies	None	Preprocessor, user's instructions, sample problems	$60 IGWMC	Package of several analytical and numerical programs
CSUPAW	Sunada Colorado State University	2-D	Unknown	Porous; homogeneous; unconfined	None	Preprocessor and postprocessor, user's instructions, sample problems	Public domain	Can calculate aquifer discharge to a stream
CRREL	Daly (1984); USACE Cold Regions Research and Engineering Laboratory	2-D	Unknown	Porous; heterogeneous; anisotropic	None	Postprocessor produces graphs of streamlines; users's instructions with example problems	Public domain	Uses Fourier and Lagurre-alpha transforms; limited boundary conditions
DREAM	Bonn and Rounds, Lewis Publishers	2-D	Unknown	Porous; heterogeneous; isotropic	None	Preprocessor and postprocessor, user's instructions, sample problems	Unknown	Computes steady-state velocities
FLOP	van den Akker (1982) RIVM, The Netherlands	2-D areal	Steady-state flow	Porous; homogeneous; confined/semiconfined	None	Preprocessor and postprocessor, user's instructions and sample problems	Unknown	FLOP-Z1 and FLOP-ZN for quasi three-dimensional solution

(Sheet 1 of 6)

Table A1 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Time Solution	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Analytic Flow Solutions (Continued)								
GWFLOW	van der Heijde (1983); IGWMC	2-D areal	Unknown	Porous; homogeneous; isotropic; confined	None	User's instructions with sample problems; preprocessor	Available	Package of seven solutions ranging from partial penetration to mounding to stream depletion
HSSWDS	Perrier and Gibson (1982); Municipal Environmental Research Laboratory	1-D vertical	Unknown	Porous; unsaturated	None	User's instructions with sample problems	Unknown	Used to estimate percolation through landfills
INFGR	Craig and Davis (1985); Oak Ridge National Laboratory (ORNL)	1-D vertical	Transient flow	Porous; unsaturated	None	User's instructions with sample problems	Unknown	Based on Green-Ampt solution
PATHS	Nelson and Schur (1980); Pacific Northwest Laboratory (PNL)	2-D areal	Transient flow	Porous; homogeneous; isotropic; confined	None	User's instructions with sample problems	Unknown	
QUICKFLOW	Rumbaugh (1991) Geraghty and Miller, Inc.	2-D areal	Steady-state and transient flow	Porous; homogeneous; isotropic	None	Graphical preprocessor, AUTOCAD- and SURFER-compatible output, user's instructions with sample problems	$500 from Geraghty and Miller	Based on solutions by Theis, Hantush and Jacob, and Strack; PC-based
SOILMOP	Ross and Morel-Seytoux (1982); Colorado State University	1-D vertical	Transient flow	Porous; homogeneous; unconfined unsaturated	None	User's instructions with example problems	Unknown	Predicts ponding time, infiltration rates, and soil moisture profiles; few users
SYLENS/ SLAEM	Haitjema (1985) Indiana University	2-D areal quasi 3-D	Steady-state and transient flow	Porous; heterogeneous; anisotropic; confined; unconfined	None	User's instructions with example problems; preprocessor and postprocessor	Unknown	Designed for regional double aquifer systems with local interconnections

(Sheet 2 of 6)

Table A1 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimen-sions	Time Solution	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Analytic Flow Solutions (Concluded)								
THWELLS	van der Heijde (1987) IGWMC	2-D	Transient flow	Porous; homogeneous; isotropic; confined	None	User's instructions with sample problems; preprocessing and postprocessing	$75 IGWMC	Handles multiple pumping and injection wells
TWODAN	Unknown	2-D	Steady flow	Porous; heterogneous; confined/unconfined	None	Preprocessor and postprocessor, user's instructions with sample problems	$525 from Scientific Software Group	Analytical element method by Strack (1989); PC based
WHPA	Blandford and Huyakorn HydroGeologic	2-D	Steady-state flow	Porous; homogeneous; isoptropic	None	Preprocessor and postprocessor, user's instructions with sample problems	$50 IGWMC	Designed for wellhead protection
Analytic Transport Solutions								
ATD123	Yeh (1981) ORNL	1-/2-/3-D	Steady-state flow; impulse, continuous, or finite duration source term	Porous; homogeneous; anisotropic	Advection; dispersion; sorption; decay	Program documentation; preprocessor and postprocessor, SURFER- compatible output	Public domain; $100 IGWMC	Uniform, steady velocities; 450 predefined options; SELECTED in EPRI Vol. 1
BEAVERSOFT	Bear and Verruijt (1987) IGWMC	1-D and 2-D	Steady and unsteady flow; unknown source term requirements	Porous; heterogeneous; confined/unconfined	Advection; dispersion	User's instructions; preprocessor and postprocessor; limited support	$60 including the text from IGWMC	Includes saltwater intrusion; analytical and numerical solutions
CHAIN	van Genuchten (1985) U.S. Salinity Laboratory	1-D	Steady-state flow; constant or degrading source term	Porous; homogeneous, saturated/unsaturated	Advection; dispersion; sorption; decay; radioactive decay	User's manual and documentation	Public domain	Based on LaPlace transforms

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Table A1 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Time Solution	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Analytic Transport Solutions (Continued)								
CRACK	Sudicky (1986) University of Waterloo	2-D	Unknown	Fractured; homogeneous; isotropic	Advection; dispersion	Preprocessor and postprocessor, user's instructions with sample problems	Unknown	
EPA-VHS	van der Heijde (1989) IGWMC	2-D	Steady-state flow, continuous source term	Porous; homogeneous; isotropic	Advection; dispersion	Preprocessor, user's instructions with sample problems	Unknown	Modified version of Domenico and Palciauskas' VHS program
FRACFLO	Gureghian (1987) Battelle Memorial Institute	1-/2-D	Steady-state flow; unknown source term requirements	Fractured; homogeneous; isotropic	Advection; dispersion; decay	User's instructions; DISSPLA graphics routines	Public domain	Available from the National Energy Software Center
GETOUT	Burkholder et al. (1976) PNL	1-D	Steady-state flow; constant source term	Porous; fractured; heterogeneous	Advection; dispersion; sorption; radioactive decay	User's instructions with sample problems	Public domain	Handles chain decay for up to three nuclides in one chain
GWMTM1/ GWMTM2	Cleary and Ungs (1978) Princeton University	1-/2-D areal or vertical	Steady-state flow; constant or degrading source term at boundary	Porous; homogeneous	Advection; dispersion; decay	Unknown	Unknown	
LTIRD	Javandel, Doughty, and Tsang (1984) Lawrence Berkeley Laboratory	1-D radial	Steady-state flow, constant source	Porous; homogeneous; isotropic; confined	Advection; dispersion	User's instructions and sample problems	$150 in SOLUTE or AGU-10 packages from IGWMC	
MYGRT	Electric Power Research Institute (EPRI)	2-D areal or vertical	Constant velocity; unknown source term requirements	Porous; homogeneous; anisotropic	Advection; dispersion; retardation; decay	Interactive, menu-driven; graphics included	$1,000 from EPRI	

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Table A1 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Time Solution	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Analytic Transport Solutions (Continued)								
NEFTRAN (NWFT/DVM)	Campbell, Longsine, and Cranwell (1981); SNL/INTERA Environmental Consultants	1-D	Steady-state flow; constant source term	Porous; fractured; heterogeneous; confined/unconfined	Advection; dispersion; diffusion; sorption; radioactive decay; dissolution; multiple chains	Unknown	Public domain	Includes salt effects on density; based on distributed velocity; requires nodal head inputs
NUTRAN	Ross et al. (1979) Analytic Science, Inc.	1-D	Steady-state flow; constant source term	Porous; heterogeneous; confined/semiconfined	Advection; dispersion; diffusion; sorption; radioactive decay; dissolution	Requires IMSL; DISSPLA software is used for plots	Proprietary	Output is amount of released radioactivity; Green's functions; requires head inputs
ODAST	Javandel, Doughty, and Tsang (1984) Lawrence Berkeley Laboratory	1-D	Steady-state flow; constant or decaying source term	Porous; homogeneous; confined	Advection; dispersion; sorption; decay	User's instructions with sample problems	$150 for the entire AGU-10 package from IGWMC	
ONE-D	van Genuchten and Alves (1982) U.S. Salinity Laboratory	1-D	Steady-state flow; unknown source term requirements	Porous; homogeneous	Advection; dispersion; sorption; decay	User's instructions with sample problems; preprocessor	$50 IGWMC	A package of five analytic solutions in a semi-infinite aquifer
PLUME	van der Heijde (1984) IGWMC	2-D areal or 3-D	Steady-state flow; variable solute injection rate	Porous; homogeneous; confined	Advection; dispersion; sorption; radioactive decay	Preprocessor and postprocessor, user's instructions with sample problems	$50 IGWMC	

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Table A1 (Concluded)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Time Solution	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Analytic Transport Solutions (Concluded)								
PLUME-2D	van der Heijde (1984) IGWMC	2-D areal	Steady-state flow; constant solute injection rate	Porous; homogeneous; confined	Advection; dispersion; sorption; decay	User's instructions with sample problems; supported	$50 IGWMC	Included in the SOLUTE package
SOLUTE	Beljin (1985) IGWMC	1-/2-/3-D	Steady-state flow; constant or slug injection	Porous; homogeneous; isotropic; confined	Advection; dispersion; sorption; decay	User's instructions with sample problems; preprocessor and postprocessor	$150 IGWMC	Package of eight models with various capabilities including PLUME2D, PLUME3D, RADIAL, LTIRD, etc.
TDAST	Javandel, Doughty, and Tsang (1984) Lawrence Berkeley Laboratory	2-D	Steady-state, uniform flow; steady or decaying source	Porous; homogeneous; isotropic; confined	Advection; dispersion; sorption	User's instructions with sample problems	$150 for entire AGU-10 package from IGWMC	
WALTON35	Walton (1984) IGWMC	1-/2-D	Steady-state flow	Porous; confined/ unconfined/ semiconfined	Advection; dispersion; heat conduction	User's instructions with sample problems; preprocessor	$50 IGWMC	
WASTE	Analytic Sciences Corporation, Inc.	1-D horizontal or vertical or 2-D areal	Unknown flow requirements; steady or transient source term	Porous; heterogeneous; anisotropic; confined/semiconfined	Advection; dispersion; diffusion; sorption; decay; ion exchange	User's instructions with sample problems	Unknown	Part of the NUTRAN package
WELFUN	Walton (1989) Lewis Publishers	2-D areal	Unknown flow requirements; slug or continuous source	Porous; confined/ unconfined/ semiconfined	Advection; dispersion; sorption; decay	Preprocessor and postprocessor, user's instructions with sample problems	Unknown	

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Table A2
Numerical Saturated Flow and Transport Models

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow and Transport Models								
AQUA	Vatnaskil Consulting Engineers	2-D	Finite element (FE)	Porous; heterogeneous; anisotropic; confined/unconfined	Advection; dispersion; sorption; decay; heat conduction	Graphic preprocessor and postprocessor, user's instructions with sample problems	$2,300 SSG for 1800 node version	PC based
ASM	University of Kassel and University of Stutgart	2-D areal	Finite difference (FD)/ particle tracking	Porous; heterogeneous, anisotropic; confined/ unconfined/ semiconfined	Advection; diffusion; decay.	Program documentation; menu-driven program with HPGL-compatible graphics	$175 IGWMC	C-based; BASIC language; Can use either RANDOM WALK or MODPATH for transport
BEAVERSOFT	Bear and Verruijt (1987) Technion and Technical University of Delft	2-D vertical	Unknown	Porous; homogeneous; anisotropic	Advection; dispersion	Documentation is in accompanying book; graphics of isochrones and pathlines	$60 IGWMC including book	BASIC language; can handle salt water intrusion
CFEST	Gupta et al. (1987) PNL/CH_2M Hill	3-D	FE	Porous; heterogeneous; anisotropic; confined/unconfined/ semiconfined	Advection; dispersion; diffusion; soption; decay; salt dissolution; heat conduction and convection	User's instructions and sample problems; preprocessor and postprocessor	Unknown	Coupled solution including density effects; used by EPA for landfills; recommended by EPRI Vol. 1; Tested in HYDROCOIN
CUMOC/ MIKERN (MOC Elite)	Illangasekare and Doll; University of Colorado	2-D	Discrete kernel/FD/ Method of Characteristics (MOC)	Porous; heterogeneous; anisotropic; confined	Advection; dispersion; sorption; decay	User's instructions with example problems	$195 SSG	C++, Macintosh only

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow and Transport Models (Continued)								
DPCT	Schwartz and Crowe (1980); University of Alberta	2-D vertical	FE/particle tracking	Porous; heterogeneous; anisotropic; unconfined	Advection; dispersion; sorption; decay	NRC report		Flow is steady state
FEMSEEP	Meiri Ebasco, Inc.	2-D areal, vertical, or axisym	FE/particle tracking	Porous; heterogeneous; anisotropic; confined/unconfined/ semiconfined	Advection; dispersion; sorption	Menu-driven pre-processor and post-processor, user's manual with test problems; graphics	$900 for flow and transport modules from SSG	No source code provided
FLOWPATH	Waterloo Hydrogeologic Software	2-D	FD/particle tracking	Porous; heterogeneous; anisotropic; confined/unconfined/ semiconfined	Advection	Preprocessor and postprocessor, user's instructions and sample problems	Unknown	Steady-state flow
FTWORK	Faust, Guswa, and Mercer (1989) GeoTrans/Savannah River Laboratory	3-D	FD	Porous; heterogeneous; confined/unconfined	Advection; dispersion; sorption; decay	User's manual with sample input/output; parameter estimator for the flow model	$700 plus $800 annual maintenance or $700 unsupported	PC based; unsteady flow, steady transport only; no rewetting of dry cells
GWTHERM	Runchal, Treger, and Segal (1979) Dames and Moore/DOE	2-D	FD	Porous; heterogeneous; anisotropic	Advection; dispersion; diffusion; sorption; decay; heat conduction and convection	Program documentation	Unknown	Includes density and temperature dependence on fluid properties
GWTRAN	Warner (1981) Colorado State University	2-D	FE	Porous; heterogeneous; isotropic; confined/unconfined	Advection; dispersion; sorption	Unknown	Unknown	Steady-state flow; decoupled transport

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow and Transport Models (Continued)								
HST3D	Kipp (1987) U.S. Geological Survey (USGS)	3-D	FD	Porous; heterogeneous; anisotropic; confined/unconfined/ semiconfined	Advection; dispersion; diffusion; sorption; decay; salt dissolution; heat conduction and convection	User's instructions and sample problems	Public domain; $40 USGS; $530 SSG with preprocessor/ postprocessor; $300 G&M with extended memory; $200 IGWMC with extended memory	PC based. Coupled solution includes density dependence on concentration, pressure, and temperature, and viscosity dependence on temperature and concentration
MAGNUM-2D/ CHAINT	Baca, Arnett, and King (1981) England et al. (1985) Rockwell (Hanford)/ Resource Management Associates	2-D 1-D for fracture	FE	Porous; fractured; heterogeneous; anisotropic	Advection; dispersion; diffusion; sorption; decay; reaction	Unknown	Public domain	Dual porosity and discrete fractures
MOC	Konikow and Bredehoeft (1978) USGS	2-D	FD/MOC	Porous; heterogeneous; anisotropic; confined/unconfined	Advection; dispersion; sorption; decay; ion exchange	Code documentation; preprocessor and postprocessor with minimal graphics	$40 USGS; $200 IGWMC with preprocessor; $340 SSG extended memory and preprocessor and postprocessor; $300 G&M with extend-ed memory ($375 Macintosh)	PC based. Decoupled flow and transport solutions. NRC version recommended by EPRI Vol. 2; SELECTED by EPRI Vol. 1; MODELCAD[386] preprocessor from G&M $750; Many add-ons like MOCGRAF, MOCINP, and MOCTIME

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Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow and Transport Models (Continued)								
MOCDENSE	Sanford and Konikow (1985) USGS	2-D vertical	FD/MOC	Porous; heterogeneous; anisotropic; confined/unconfined	Advection; dispersion; sorption; decay; ion exchange	Code documentation; minimal data needs; preprocessor and postprocessor	$40 USGS; $120 IGWMC with no support; $320 SSG extended memory	Same as MOC but includes density-dependent flow for simulating saltwater intrusion
PINDER	Pinder (1973) Princeton University	3-D	FE	Porous; heterogeneous; anisotropic	Advection; dispersion; sorption	Unknown	Unknown	Coupled transport and flow solutions
PORFLOW-II	Runchal (1985) Analytic and Computational Research	2-D areal, vertical, or radial	FD	Porous; heterogeneous; anisotropic	Advection; dispersion; heat conduction and convection	Preprocessor and postprocessor, user's instructions and sample problems	Unknown	
PTC	Babu et al. (1984) Princeton University	3-D	FE within layers, FD between layers	Porous; heterogeneous; anisotropic; confined/unconfined	Advection; dispersion; sorption	Unknown	Unknown	Uncoupled flow and transport
RANDOMWALK (TRANS)	Prickett, Naymik, and Lonnquist (1981) Illinois State Water Survey	2-D areal	FD/RANDOM WALK	Porous; heterogeneous; anisotropic; confined/unconfined; incompressible	Advection; dispersion; diffusion; sorption; decay	Preprocessor and postprocessor, program documentation; code annotation; no graphics	Available; $100 IGWMC either PC or mainframe	SELECTED by EPRI Vol. 1 and evaluated in EPRI Vol. 3; MODELCAD[386] preprocessor from G&M $750
ROBERTSON2	Bredehoeft and Pinder (1973) USGS	2-D areal	FD/MOC	Porous; heterogeneous; anisotropic	Advection; dispersion; sorption; ion exchange; radioactive decay	Unknown	Public domain	Coupled flow and solute transport solutions

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Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow and Transport Models (Continued)								
SALTRP	Frind and Trudeau (1980) Stone and Webster	2-D areal	FE	Porous; confined	Advection; dispersion; diffusion; salt dissolution	Unknown	Proprietary	
SEFTRAN	Huyakorn (1984) GeoTrans, Inc.	2-D areal, vertical, or axisym	FE	Porous; fractured; heterogeneous; isotropic; confined/ unconfined	Advection; dispersion; diffusion; sorption; decay; heat conduction; convection	User's instructions and examples; pre-processor and post-processor	$500 unsupported from GeoTrans	PC version; available, but no longer on GeoTrans' published list of codes
SHALT	Pickens and Grisak (1979) Environment Canada	2-D areal or vertical	FE	Porous; heterogeneous; anisotropic; confined/unconfined	Advection; dispersion; diffusion; sorption; decay; reactions; ion exchange; heat transfer	Unknown	Unknown	Coupled solute, heat, and liquid transport
SWENT	INTERA Environmental Consultants (1983)/Office of Nuclear Waste Isolation (ONWI)	3-D	FD	Porous; heterogeneous; anisotropic; confined; compressible	Advection; dispersion; diffusion; sorption; decay; radioactive chain decay; salt dissolution; heat conduction and convection	User's instructions; postprocessor for sensitivity analyses of steady-state problems; verification documentation	Unknown	Coupled solution that includes a well-bore model; SELECTED by EPRI Vol. 1; Tested in HYDROCOIN

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Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow and Transport Models (Concluded)								
SWICHA	Lester GeoTrans, Inc.	3-D	FE	Porous; heterogeneous; anisotropic	Advection; dispersion; sorption; decay	User's manual, example data sets, preprocessor	Proprietary; $700 plus $800 annual maintenance or $500 unsupported from GeoTrans; $200 from IGWMC unsupported	Density-dependent flow for seawater intrusion; PC based; executable only
SWIFT III/ SWIFT/386/ SWIFT/486	Ward, Reeves, and Duda (1984) GeoTrans, Inc./ Sandia National Laboratory (SNL)	3-D	FD	Porous; fractured; heterogeneous; anisotropic; confined/unconfined/ semiconfined; variable porosity	Advection; dispersion; diffusion; sorption; decay; radioactive chain decay; salt dissolution; heat conduction and convection	Postprocessor, documentation, and sample problems; 2-D printer-plotter contour mapping; extensive error checking	SWIFT III $2,500. SWIFT/386 either $1,000 plus $800 annual maintenance or $800 unsupported from GeoTrans. SWIFT/486 $1,800 supported or $800 unsupported from SSG	SWIFT/386 and 486 are PC based. Discrete fractures or dual porosity; coupled, variable density transport; tested in HYDROCOIN; 30,000 cells maximum
TRAFRAP-WT	Huyakorn, White, and Wadsworth (1987) GeoTrans, Inc.	2-D areal	FE	Porous; fractured; heterogeneous; anisotropic; semiconfined/ unconfined	Advection; dispersion; diffusion; adsorption; decay; reactions	User's instructions and examples; no preprocessor or post-processor	$250 IGWMC with extended memory	PC based. Discrete fractures and dual porosity. Can handle 1,000 elements or 1,200 nodes, maximum

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
				Flow Models				
AQ/BASIC GWF	Verruijt (1981) Technical University of Delft	2-D areal	FE	Porous; heterogeneous; isotropic; confined/ unconfined	None	Preprocessor and postprocessor including graphics, user's instructions with sample problems	Unknown	
AQ-FEM	National Institute of Public Health, The Netherlands	2-D areal/ quasi 3-D	FE	Porous; heterogeneous; anisotropic	None	Preprocessor and postprocessor, user's instructions and sample problems	Unknown	
AQU-1	Rushton and Redshaw (1979) University of Birmingham	2-D areal	FD	Porous; heterogeneous; anisotropic; confined/ semiconfined	None	User's instructions with sample problems	Unknown	
AQUIFEM-n	Townley and Wilson (1980) MIT	2-D areal/ quasi 3-D	FE	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	User's instructions; sample problems	$1,100 for 1,000 node 2-D, PC-based version from SSG	
COOLEY	Cooley (1974) DRI, University of Nevada	2-D areal or vertical	FE	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	Good documentation	Public domain	Used by Dames and Moore and extensively by DRI; constant thickness; 2,500 nodes maximum
DISIFLAQ	Bemey (1981) United Nations	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; isotropic; confined/ semiconfined	None	User's instructions with sample problems	Unknown	Only two layers may be simulated

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow Models (Continued)								
FE3DGW	Gupta, Cole, and Bond (1979) PNL/ONWI	3-D	FE	Porous; heterogeneous; anisotropic; confined/unconfined/ semiconfined; compressible	None	User's manual; consistency checks; graphics; automatic grid generator; many references	Public domain	This is the flow solver for CFEST; SELECTED in EPRI Vol. 1; Tested in HYDROCOIN; 2,560 nodes
FLOWNET		2-D vertical	FD	Porous; heterogeneous; anisotropic; confined/ unconfined	None	Preprocessor and postprocessor, user's instructions with sample problems	Unknown	Steady-state flow
FLUMP	Neuman, Narasimhan, and Witherspoon (1977) University of Arizona	2-D areal or vertical	FE	Porous; heterogeneous; anisotropic	None	Unknown	Public domain	
FRESURF1/2	Neuman and Witherspoon (1971) University of Arizona	2-D areal or vertical	FE	Porous; heterogeneous; anisotropic	None	User's instructions; example problems	Public domain	Computes the seepage face in vertical mode
GWFL3D	Walton (1989) Lewis Publishers	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; confined/ unconfined/ semiconfined	None	Preprocessor and postprocessor, user's instructions with sample problems	Unknown	
GWFLOW	Warner (1981) Colorado State University	2-D areal	FE	Porous; heterogeneous; anisotropic; confined/ unconfined	None	Preprocessor and postprocessor including grid generator and graphics. User's instructions with sample problems	Public domain	

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow Models (Continued)								
INTERSAT	Voorhees ESE/Hydrosoft	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	Integrated package with data manager, grid generator and graphics and a surface water package	$600 SSG	81,000 node maximum
JBD2D/3D	Bredehoeft (1991) USGS	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; anisotropic	None	Source code; user's instructions; example problems	Public domain; $40 USGS; $50 IGWMC version uses math coprocessor	
MICROFEM		2-D areal/ quasi 3-D	FE	Porous; heterogeneous; anisotropic; confined	None	User's manual; preprocessor and postprocessor including grid generator and graphics	$960 IGWMC including source code, unsupported	PC based; PASCAL language; steady state only; 3,000 nodes or 6,000 elements
MODFE	USGS	2-D	FE	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	Preprocessor and postprocessor, user's instructions and sample problems	Public domain; $40 USGS; $350 extended memory version from SSG	

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow Models (Continued)								
MODFLOW	McDonald and Harbaugh (1988) USGS	3-D	FD	Porous; heterogeneous; anisotropic; confined/ unconfined; semiconfined	None	Good documentation and support; preprocessor and postprocessor; many add-on packages	Public domain; $40 USGS; $339 SSG with extended memory and utilities; $300 G&M with extended memory ($375 for Macintosh); $350 IGWMC extended memory	PC based. MODLMAKR preprocessor by Microcode $295; MODELCAD[386] preprocessor by G&M $750. Included in the GMS
PLASM	Prickett and Lonnquist (1971) Illinois State Water Survey	2-D areal or vertical or quasi 3-D	FD	Porous; heterogeneous; confined/unconfined/ semiconfined	None	User's instructions with sample problems; preprocessor and postprocessor; supported	Public domain; $120 IGWMC; includes PLASM85, CONPLASM, and UNCPLASM	PC based
SGMP	Boonstra and de Ridder (1981) International Institute for Land Reclamation and Improvement, The Netherlands	2-D areal	FD	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	User's instructions with sample problems	Unknown	Nonrectangular cells
SLAM	Aral (1990) Georgia Tech	2-D areal/ quasi 3-D	FE	Porous; heterogeneous; confined/ unconfined/ semiconfined	None	User's instructions with sample problems	Unknown	Steady-state flow

Table A2 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Flow Models (Concluded)								
UNSTEADY-FLOW	Aral (1990) Georgia Tech	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; confined/unconfined/ semiconfined	None	User's instructions with sample problems	Unknown	
USGS-2D	Trescott, Pinder, and Larson (1976) USGS	2-D areal or vertical	FD	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	User's instructions and example problems; no preprocessor and postprocessor	Public domain; $100 IGWMC	One of the basis codes for MODFLOW; PC version
USGS-3D	Trescott (1975) USGS	3-D	FD	Porous; heterogeneous; anisotropic; confined/ unconfined	None	User's instructions and example problems; no preprocessor or post-processor; detailed mass balance check	Public domain; $100 IGWMC	Can be run in quasi 3-D; widely used; basis code for MODFLOW; Mainframe version only; tested in HYDROCOIN
V3	Prickett and Lonnquist (1971) Illinois State Water Survey	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	Unknown	Public domain	Leakage between layers is assumed steady; widely used
VTT	Bond, Newbill, and Gutnecht (1981) PNL	2-D areal/ quasi 3-D	FD	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	None	Code documentation, preprocessor and postprocessor	Public domain	Uniform grid spacing; SELECTED by EPRI Vol. 1
Transport Only Models								
GWPATH	Shafer (1982) Illinois State Water Survey	2-D areal or vertical	Unknown	Porous; heterogeneous; anisotropic	Advection	Graphics of capture zones and pathlines	Unknown	PC based; steady-state head distribution

(Sheet 11 of 12)

Table A2 (Concluded)

Model Name	Author or Contact and Institution (with reference if known)	Dimen-sions	Solution Method	Matrix Properties	Transport Processes Treated	Supporting Documentation or Software	Availability	Comments
Transport Only Models (Concluded)								
GWTR3D	Walton (1989) Lewis Publishers	2-D areal	RANDOM WALK	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	Advection; dispersion; sorption; radioactive decay	Preprocessor and postprocessor, user's instructions with example problems	Unknown	
INTERTRANS	Voorhees ESE/ Hydrosoft, Inc.	3-D	RANDOM WALK	Porous; heterogeneous; anisotropic	Advection; dispersion	Preprocessor and postprocessor, user's instructions with sample files	$500 from SSG for 81,000 nodes	No source code
MODPATH	Pollack (1989) USGS	3-D	Particle tracking	N/A	Advection	User's instructions; preprocessor and postprocessor for data; produces SURFER-compatible files	Public domain; $40 USGS; $300 G&M with extended memory	Translator in MODELCAD[386] from G&M
MT3D	Zheng (1990) S. S. Papadopulos and Associates	3-D	Particle tracking/FD	N/A	Advection; dispersion; diffusion; sorption; radioactive decay or biodegra-dation	User's instructions with example problems	Available; $495 (includes MODFLOW/ mt from SSP&A)	Uses adaptive local grid refinement methods; Can be used with other models, but was designed to be used with MODFLOW. Translator in MODELCAD[386]. Included in the GMS by the end of FY95
RAND3D	Prickett and Koch (1990) Koch and Associates	3-D	RANDOM WALK	N/A	Advection; dispersion; diffusion; sorption; decay	Preprocessor and postprocessor, user's instructions with example problems	Unknown	PREMOD3D converts MODFLOW. Output into velocity vectors for RAND3D. Will be included in the GMS by the end of FY97

Table A3
Numerical Saturated and Unsaturated Flow and Transport Models

Model Name	Authors	Dimen-sions	Solution Method	Major Processes	Matrix Properties	Transport Processes Treated	Comments
HYPE	Wagner et al. (1984)	2-D vertical	FE flow MOC and FD transport; linear quadrilateral elements	Advection; coupled saturated and unsaturated zones	Porous; heterogeneous, anisotropic	Linear partition equilibrium sorption degradation in liquid and solid phases (first order)	Uncoupled flow and transport, constant density, pressure saturation relationship based on Campbell's relationship. EPA's KER Lab distribution
SUTRA	Voss, C. I. (1984)	2-D vertical	FE	Advection dispersion and diffusion; coupled saturated and unsaturated zones; both energy and solutes	Porous; heterogeneous and anisotropic	Linear partition equilibrium sorption, degradation and chemical reactions	Coupled flow and transport, variable density; user provides the pressure saturation relationships. IGWMC distribution $200
SATURN	Huyakorn, P. (1982)	2-D vertical	FE linear rectangular and triangular elements	Advection, dispersion, diffusion; coupled saturated and unsaturated zones	Porous, heterogeneous, anisotropic	Linear partition equilibrium sorption, degradation (first order) chemical reactions	Uncoupled flow and transport, constant density; user provides the pressure satuation relationships
FEMWATER/ FEMWASTE	Yeh, G. T., and Ward, D. S. (1981) and (1980)	2-D vertical	FE quadrilateral bilinear and triangular elements	Advection, hydrodynamic dispersion and diffusion; coupled saturated and unsaturated zones	Porous, heterogeneous and discontinuos media	Linear partition equilibrium sorption, degradation (first order), and sources/sinks	Uncoupled flow and transport, constant density; user provides relationship or data for the pressure saturation relationship
3DFEMWATER-3DLEWASTE	Yeh, G. T., and Cheng, J. R. (1994)	3-D	FE hexahedral, triangular prism, and tetrahedral elements	Advection, hydrodynamic dispersion, and diffusion; coupled saturated and unsaturated zones; Lagrangian-Eulerian transport	Porous, heterogeneous and anisotropic media	Linear partition equilibrium, Langmuir and Freunlich nonlinear isotherms, point sources/sinks that are spatially and temporally dependent	Uncoupled flow and transport; user provides data for the pressure saturation relationship; IGWMC, Pennsylvania State University; Included in the GMS
SESOIL	Bonazountas, M., and Wagner, J. M. (1981)	1-D vertical	Completely mixed compartments	~advection diffusion water balance; unsaturated soil column	Soil column	Linear partition equilibrium sorption, degradation, hydrolysis, and complexation	Water movement in unsaturated soil with pollutants in equlibrium between the solid, liquid, and gas phases

(Continued)

Table A3 (Concluded)

Model Name	Authors	Dimensions	Solution Method	Major Processes	Matrix Properties	Transport Processes Treated	Comments
PRZM	Carsel et al. (1984)	1-D vertical	FD and MOC in the new release	Advection diffusion water balance; runoff; unsaturated soil column	Soil column	Linear partition equilibrium sorption, degradation, hydrolysis, and plant uptake	Water movement in unsaturated soil based on the concepts of field capacity and wilting point. Developed for pesticide transport from agricultural applications
RUSTIC	Dean et al. (1989)	1-D unsaturated vertical 2-D saturated vertical, horizontal, and/or axisymmetric	FD and MOC in soil/root zone FE unsaturated zone	Advection, dispersion, and diffusion; runoff, evapotranspiration, and infiltration; unsaturated and saturated zones not coupled; unconfined and confined saturated zones	Soil column; porous media	Linear partition equilibrium sorption and degradation (first order lumped); plant uptake in the root zone	Water movements in the upper zone are based on the concepts field capacity and wilting point. Uncoupled saturated and unsaturated flow; coupled flow and transport; constant density. Three models: PRZM, VADOFT, and SAFTMOD
FLAMINCO		3-D	FE	Advection, dispersion, and diffusion; coupled unsaturated and saturated zones	Porous media; heterogeneous	Linear partition equilibrium sorption and degradation	Water flow and solute transport in saturated and unsaturated zones
VAM2D	Huyakaron, P. S. (1988)	2-D vertical, horizontal, and/or axisymmetric	FE	Advection and dispersion; coupled unsaturated and saturated zones	Porous media; heterogeneous; anisotropic	Linear partition equlibrium sorption and degradation	Water flow and solute transport, recharge infiltration and highly nonlinear soil moisture relationships
VAM3D	Huyakron, P. S. (1988)	3-D vertical, horizontal, and/or axisymmetric	FE	Advection and dispersion; coupled unsaturated and saturated zones	Porous media; heterogeneous; anisotropic	Linear partition equlibrium sorption and degradation	Water flow and solute transport
VS2DT	Lappala, Healy, and Weeks (1987)	2-D vertical cross section, x-z or axially symmetric 3-D	FD	Advection, dispersion; coupled unsaturated and saturated zones	Porous media; heterogeneous; anisotropic; direction of flow must coincide with coordinate axes	Ion-exchange and degradation	Water flow and solute transport
UNSAT1	van Genuchten, M. Th. (1985)	1-D vertical	FE	Advection dispersion in unsaturated soil column	Porous media; heterogeneous	NA	Water flow

Table A4
Geochemical and Hydrochemical Models

Model Name	Authors	Type	Solution Technique	Adequate Thermodynamic Database	Important Processes	Transport Processes Treated	Availability	Comments
CHEMIST	Deland (1967)	Speciation	Gibbs free energy minimization		Speciation, gas-phase equilibrium (GPE)	NA		
EQUILIB	Morrey (1978)	Speciation	Back substitution; ligand projection method	NBS, Helgenson's database, and others	Speciation, hydration, ion interaction, reduction/ oxidation (R/O), GPE, and precipitation/ dissolution (P/D)	NA		No adsorption capability
EQ3/EQ6	Wolery (1979)	Speciation reaction path	Finite difference Newton-Raphson	Helgenson's database	Speciation, hydration, ion interaction, R/O, GPE, P/D, and kinetics	NA		No adsorption capability
GEOCHEM	Sposito and Mattigod (1979)	Speciation	Newton-Raphson	USGS and others	Speciation, hydration, ion interaction, R/O, GPE, adsorption/ desorption (A/D), and P/D	NA		No kinetics, database with many species of interest for soil science
GEOCHEM-PC	1988							PC version
PHREEQE	Parkhurst et al. (1980)	Reaction path	Back substitution Newton-Raphson	WATEQ2 database	Speciation, hydration, ion interaction, R/O, GPE, P/D, A/D and pseudo kinetics	NA	IGWMC USGS	Limited adsorption model, no rate constants in the kinetics model
PHRQPITZ	Plummer et al. (1988)	Specific interaction model; speciation and mineral saturation in high concentration electrolyte solutions		WATEQ plus Pitzer interaction parameters for many inorganic salts	Speciation, ion interaction at high electrolyte concentrations, irreversible reactions, and temperature effects	NA	USGS	Dilute to highly concentrated mixed-electrolyte solutions, limited data outside of seawater salts

(Sheet 1 of 3)

Table A4 (Continued)

Model Name	Authors	Type	Solution Technique	Adequate Thermodynamic Database	Important Processes	Transport Processes Treated	Availability	Comments
PHREEQM	Appelo and Willemsen (1987)	Geochemical mass transport 1-D	Back substitution Newton-Raphson	WATEQ2	Speciation, chemical mass transfer, R/O, A/D	Hydrodynamic advection and dispersion	IGWMC	Mixing cell model; simple flow modeling-steady-state 1-D flow fields; based on PHREEQE
BALANCE	Parkhurst, Plummer, and Thorstenson (1982)	Reaction model	Gaussian Elimination	NA	Mineral/water interactions, R/O	NA	IGWMC	Derive balance equations
NETPATH		Net geochemical mass-balance reactions	Gaussian Elimination	WATEQ	Mineral/water interactions, R/O, isotopic composition	NA, flow path	IGWMC	User defines the geochemical system, uses WATEQF for possible reactions
CHEMTRN	Miller and Benson (1983)	Geochemical transport and chemical equilibrium	Mixed-differential-algebraic model		Speciation, ion exchange, A/D, and P/D	Advection dispersion		
THCC		Nonisothermal version of CHMTRN						
MINTEQ	Felmy, Girvin, and Jenne (1983)	Speciation	Newton-Raphson ligand projection method	WATEQ3 database	Speciation, hydration, ion interaction, R/O, GPE, A/D, and P/D	NA		No kinetics lacks preprocessor
MINTEQA2/ PRODEFA2 version 3.0	Allison et al. (1990)	Speciation	Newton-Raphson ligand projection method	WATEQ3 database	Speciation, hydration, ion interaction, R/O, GPE, A/D, and P/D	NA	USEPA Athens	Extensive database that includes many heavy metals; updated regularly
MININR		Speciation		WATEQ3 database				

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Table A4 (Continued)

Model Name	Authors	Type	Solution Technique	Adequate Thermodynamic Database	Important Processes	Transport Processes Treated	Availability	Comments
MEXAMS	Felmy et al. (1984)	Speciation transport	Newton-Raphson	WATEQ3 database	Speciation, hydration, ion interaction, R/O, GPE, A/D, and P/D	Advection steady state	USEPA athens	Coupled MINTEQ with EPA's EXAMS model
TRANSCHEM	Rafal and Sanders	Speciation	Newton-Raphson		Speciation, GPE, R/O, A/D, and P/D	NA		Temperature and pressure effects
WATEQF	Plummer, Jones, and Truesdell (1976)	Chemical equilibrium		WATEQ	Speciation, R/O	NA	USGS	No adsorption capability
WATEQ4F		Speciation	Back substitution	WATEQ	Speciation, hydration, ion interaction, R/O, GPE, and P/D	NA	USGS IGWMC	No adsorption capability
MINEQL+	Schecher and McAvoy (1991)	Speciation, precipitation, pH, and adsorption	Newton-Raphson	MINTEQA1 and MINEQL databases	Speciation, R/O, adsorption	NA	Environmental Research Software	Advanced interface
SOILCHEM	Sposito and Coves (1988)	Speciation	Newton-Raphson	USGS, WATEQ	Speciation, GPE, A/D, R/O, and P/D	NA		Based on GEOCHEM and REDEQL2
FASTCHEM		Geochemical flow and transport in unsaturated and saturated zones	2-D FE particle tracking Newton-Raphson iteration technique	WATEQ3 database	Speciation P/D, A/D	Advection dispersion (Markov method)	EPRI	Coupled SATURN with MINTEQ
HYDRO-GEOCHEM	Yeh and Tripathi (1991)	Geochemical transport in unsaturated and saturated zones	2-D FE for hydrologic transport Newton-Raphson and/or modified bisection method for equilibrium	User provides equations and thermodynamic data	Speciation, hydration, ion interaction, R/O, P/D, A/D	Advection dispersion	Author at Pennsylvania State University	Transport is based on the FEMWASTE model; sequential iteration model

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Table A5
Flow and Transport Models for Fractured or Structured Media

Model Name	Authors	Dimensions	Solution Technique	Fracture-Matrix Model	Transport Processes Treated	Comments
BIM, BIM2D, BIM3D, FRACGEN	University of Arizona	3-D or 2-D	Boundary Integral Method	Discrete fracture (DISC), dual-porosity (bi-continuum) (DUAL)	Linear equilibrium adsorption. Diffusion into matrix	Unsaturated, fractured, porous media. Transient. Solute travel times and breakthrough curves are estimated by integrating inverse velocity over streamlines and summing. FRACGEN generates synthetic network
CRACK	Sudicky and Frind (1982), Sudicky (1986), University of Waterloo	1-D	AN (package of 4)	DISC (single) or DUAL; diffusive exchange	Matrix diffusion with/without fracture dispersion	Four analytical models: (1,2) single fracture with matrix diffusion, w/wo dispersion in fractures; (3) single fracture w/ matrix diffusion and radial diverging flow; (4) transport in parallel fracture network with matrix diffusion
FLASH (flow)/ FLAME (transport)	Idaho Nat. Engr. Lab.	2-D vertical or areal	Finite-element (FEM)	DISK, DUAL	Heat conduction in vadose	Variably saturated; Richard's equation. Transient. Fractured porous media
FLOWS	Noorishad and Mehran (1982), Lawrence Berkeley Lab (LBL)	2-D	FEM (Galerkin, UW)	DISC	Adsorption, Decay	Isotropic, heterogeneous, variably saturated
FRACFLOW	Sagar (1981) Analy. and Comp. Res.; now at SW Res. Inst.	2-D in porous matrix; 1-D in fractures	Integrated finite difference (IFD)	DUAL; arbitrary fracture orientation	1st-order decay. Adsorption Heat conduction and convection	Density-dependent, steady-state or unsteady flow in fractured, confined aquifers. Media consolidation
FRACMAN/ MAFIC	Dershowitz, Geier, and Lee (1991); Miller (1990) Golder Assoc.	3-D: 2-D for fracture elements, 1-D for fracture-matrix exchange	FEM w/ conj. grad. solver; Interactive, stochastic concep-tualization. Particle tracking	DISC or DUAL	Particle tracking for transport in fractures	FracMan is a discrete fracture modeling system including an interface for interactive, stochastic, fracture conceptualization and a flow and transport module. Applied to Stripa site in Sweden. Code available from Dershowitz (Golder)
FRACPORT (FRACtured PO-Rous medium Transport)	DeAngelis, Yeh, and Huff (1984) Oak Ridge National Laboratory	3-D	Integrated Compartmental Model	DUAL. Separate calculation of transport in fracture (fast) and matrix (slow)	Adsorption. Decay	Transport only; requires independent determination of the velocity field. Saturated, fractured, porous media

(Sheet 1 of 6)

Table A5 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Fracture-Matrix Model	Transport Processes Treated	Comments
FRACSL	Clemo and Hull (1983); Miller (1983); Idaho Nat. Engr. Lab.	2-D	Finite difference (FD)	DISC	Diffusion. Heat conductance and convection	Steady-state, solute and heat transport in fractured porous media
FRACSOL	Grisak and Pickens (1981); INTERA	1-D	AD	DUAL; regular spacing	Diffusion	Simple model. Limited applicability
FRACT	Pickens and Grisak (1981a,b); INTERA	1-D	FEM	DUAL	Adsorption, ion exchange. Decay	Linear fractures with diffusion into matrix
FTRANS (fracture Flow, Thermal, and RAdioNuclide Solute transport)	Huyakorn (1983) for Battelle	2-D (areal, vert., or axisym.) for fractures; 1-D within matrix	FEM, UW for fractures	DUAL (fractured) or equivalent porus medium (EPM) (unfractured)	Adsorption, diffusion. 1st-order decay. Heat conduction. Leakage	Proprietary. Transient. Confined or semiconfined. Variable density flow and transport
GREASE2		2-D	FEM	DUAL (fractured) or EPM (unfractured)	Adsorption. Leakage from confining layers. Heat conduction	Proprietary. Transient. Heterogeneous, multilayered media. Density dependent flow
MAGNUM/2D	Baca, Arnett, and King (1981); Rockwell Hanford Operations	2-D (vert.) or 3-D (axisym.) for matrix; 1-D for fractures	FEM	DUAL or DISC (as isoparametric line elements)	Multicomponent (parent, 2 daughter) transport in fractures only. Decay. Equilib. sorption. Heat transport	Transient. May be linked to radionuclide chain decay module CHAINT. Support programs for grid generation, and postprocessing visualization. Public domain
MOTIF (Model Of Transport In Fractured/ porous media)	Guvanasen (1984); Source: T. Chan, Atomic Energy Canada, Ltd., Whiteshell Nuc. Res. Est.; Pinawa, Manitoba	3-D	FEM	DISC; sparse fractures in low permeability media	Diffusion into matrix. Transport of brine and single radionuclide. Adsorption, ion exchange. Decay runs. Heat convection and conduction	Saturated or unsaturated flow with hysteresis; capillary forces. Compressible media. Applied to radionuclide transport modeling
MULKOM	Pruess (1983); LBL	2-D	IFD	DUAL (fractured), EPM (unfractured)	Multicomponent and heat transport. Silica dissolution or pptn	Multiphase fluid (sat/unsat.). Compressible media. Phase change (evapo-transportation; gas solubility). Basis of TOUGH

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Table A5 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Fracture-Matrix Model	Transport Processes Treated	Comments
NEFTRAN (NEtwork Flow and TRANsport)	Longsine, Bonano, and harlan (1987); Sandia National Laboratories	1-D into a 3-D network	FD with particle tracking	DISC, DUAL	Matrix diffusion. Transport in fractures ("legs") only	Saturated. Steady state
NETFLO/ NETRANS	University of Quebec, Canada	2-D fracture network	FE with particle tracking; Stochastic network generation	DISC	Transport in fractures only	Four programs: (1) NETWRK is a 2-D, MONTE CARLO, fracture network generator; (2) APEGEN generates aperture data; (3) NETFLO is FE code to compute steady-state, macroscopic flow parameters and statistics; (4) NETRANS uses particle tracking to estimate travel times. Saturated. Steady state
PORFLO	Kline, Runchal, and Baca (1983)	2-D, vertical or axisymmetric	IFD	EPM	Sorption. Decay. Density-controlled (conc.) flow. Dissolution (leaching). Heat generation, conduction, convection	Proprietary code (Kline; Boeing Comp. Serv., Richland, WA). Transient. Anisotropic, heterogeneous media; confined or semiconfined. Multiphase flow (water and vapor)
PORFLOW-3D	Runchal (1985, 1987)	3-D	IFD	EPM	Sorption. Decay. Density (conc.) controlled flow. Dissolution (leaching). Heat transport	Proprietary code (Runchal; Bel Air, CA). Transient. Anisotropic, heterogeneous media; confined or semiconfined. Multiphase conditions (water and vapor). Extensively verified
ROCMAS -H (flow), -HM (flow-stress), -HS (C-D transport), -THM (thermo-mech.)	Noorishad, Ayatollahi, and Witherspoon (1981); Noorishad and Menran (1982); LBL	2-D	FEM	DUAL	-HS: Adsorption; Decay; Reactions	Four submodels: -H is flow only; -HS is solute transport; -HM is for stress modeling; and -THM is a thermo-mechanical model
SEFTRAN (Simple and Efficient Flow and TRANsport model)	Huyakorn et al. (1988) GeoTrans, Inc.	2-D, vertical, areal, or axisymmetric	FEM; line elements for fractures (or rivers)	EPM (granular medium) or DISC (line elements)	Linear equil. adsorption. 1st-order degradation. Heat transport.	Transient. Confined or unconfined; isotropic heterogeneous media

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Table A5 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Fracture-Matrix Model	Transport Processes Treated	Comments
SHALT	Pickens and Grisak (1979), Intera Tech., Inc.	2-D	FEM	EPM (uncertain)	Lin. eq. adsorption, ion exchange. 1st-order decay. Heat conduction and convection	Fractured, anisotropic, heterogeneous media. Confined or unconfined. Sat./Unsat. Aquitard leakage
STAFF2D (Solute Transport And Fracture Flow in 2 Dimensions)	Huyakorn (1988) HydroGeologic, Inc.	2-D, vertical, areal, or axisymmetric	FEM	EPM (granular medium) or DISC (intricate network to a few discrete fractures)	Linear equil. adsorption. 1st-order degradation	Transient. Confined or unconfined; aquitard leakage, infiltration
SWIFT III	Ward, Harrover, and Vincent, GeoTrans; Reeves et al. (1986a,b; II), SNL; Reeves and Cranwell (1981; I), SNL	3-D cartesian, 2-D radial; 1-D in matrix	FD	DUAL or DISC in fracture zone	Adsorption (equilib. linear or Freundlich). Radionuclide leaching and chain decay	Transient. Confined or unconfined, saturated flow. Anisotropic, heterogeneous media. Conc.-dependent fluid density. Well documented
TOUGH (Transport of Unsaturated Groundwater and Heat)	Pruess, Tsang, and Wang (1985), Pruess (1986); LBL	2-D matrix, 1-D fracture	IFD	DUAL	Phase change (vapor). Water and air phase flows. Heat conduction and diffusion. Silica dissolution-pptn.. Adsorption	Can model transient strongly, heat-driven flows of water and air (vapor). Verified against analytical solutions and applications. Evolved from MULKOM
TOPSAC (Total Systems Performance Assessment Code)	Wilson and Dudley (1985) SPECTRA Res. Inst. for SNL	1-D	FD	DUAL; parallel continua coupled by leakage term	Transport calculated separately for fractures and permeable matrix. Adsorptive retardation. Radionuclide decay	Research code. Unsaturated, fractured, porous media. Describes advective transport in both fractures and matrix
TRACR3D	Travis (1984) Los Alamos National Lab (LANL)	3-D	FD	EPM	Multicomponent Adsorption Decay	Transient. Two-phase flow (air, water). Deformable, heterogeneous, variably-saturated, porous and/or fractured media. Rad. waste model

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Table A5 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Fracture-Matrix Model	Transport Processes Treated	Comments
TRAFRAP-WT (TRAnsport in FRAtured Porous media with Water Table boundary conditions)	Huyakorn, White, and Wadsworth (1987) for International Grand Water Modeling System (IGWMC)	2-D	FEM	DUAL and/or DISC; fracture advection, matrix diffusion; EPM for unfractured	Radioactive decay chain reactions	Public domain; supported by IGWMC. Transient. Anisotropic, heterogeneous, multilayered, fractured or granular porous media. Confined or unconfined
TRUCHN/ZONE	Neretnieks and Rasmuson (1984), Royal Inst. of Tech., Sweden	2-D, axisymmetric	IFD	Multiple interacting continua (MINC) or DUAL	Diffusion into matrix blocks of various sizes and shapes	Research code. A-D in strongly fissured media. Highly variable flow velocities
TRUMP	Edwards (1972)	2-3 ('multi')	IFD	EPM or DISC	Decay. Diffusion. Heat transport	Transient or steady state; Contact: Rasmuson at Dept. of Chem. Engr., Royal Inst. of Tech., Stockholm, Sweden
WAFE	Travis (1986); LANL	2-D	IFD	EPM	Adsorption (4 models); 8 species. Decay. Heat transport	Anisotropic, heterogeneous, saturated or unsaturated media. Two phases (water and vapor)
None	Cacas, LeDoux, de Marsily et al. (1990); *Ecole des Mines de Paris*, France	3-D	Part. tracking in pipe network; stochastic	DISC; fractures simulated as a network of pipes	Particle tracking method simulates only advection and dispersion (in fracture, global tortuosity "retardation")	Research code. Network of disk-shaped fractures is generated stochastically to emulate field information
None	Glover (1987)	3-D	FEM for flow; AN for mass transfer	DUAL; parallel fracture system	Diffusion into matrix (low permeability, high porosity)	Developed for application to transport in fractured, oil shale systems
None	Narashima and Pruess (1988); Pruess and Narashima (1982)	3-D globally, 1-D diffusion	IFD	MINC	Diffusion (matrix blocks)	Research code. Global flow along fractures (internodal line elements). Multiple hierarchical levels of continua. Modified TRUMP
None	Schwartz and Smith (1985, 1987); Schwartz, Smith, and Crowe (1983); Smith and Schwartz (1993)	2-D, 3-D	Particle tracking. Stochastic submodel to estimate continuum dispersive behavior	DISC	Advection and dispersion only	Research code. MONTE CARLO simulations of orthogonal fracture networks yield statistical description of dispersion at the continuum REV scale

Table A5 (Concluded)

Model Name	Authors	Dimensions	Solution Technique	Fracture-Matrix Model	Transport Processes Treated	Comments
None	Tsang and Tsang (1987); Tsang, Tsong, and Hale (1991)	3-D network of 1-D equations	Stochastic/Analytical	DISC; interconnecting channels model	Advection and dispersion only	Research code. Gamma function for aperture widths
None	van Genuchten and Dalton (1986)	1-D	Analytical	DUAL (mobile/immobile region dichotomy)	Inter-region, mass transfer coefficient (α)	Research code. Solutions for spherical, regular block, and cylindrical immobile regions, and hollow cylindrical macropores. Homogeneous immobile regions

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Table A6
Compositional Multiphase Flow and Transport Models

Model Name	Authors	Dimensions	Solution Technique[1]	Phases	Matrix Properties	Number of Components	Transport Processes Treated	Comments[2]
GASOLINE	Baehr (1987) Corapcioglu and Baehr (1987)	1-D, vertical	Finite difference (FD)	***W***, *O* (residential), *V*	Porous, homogeneous	1	*W-O-V* equilibrium; linear adsorption, redox reactions, biodegradation	Research code
KOPT/OILENS (Kinematic Oily Pollutant Transport) and TSGPLUME (Transient Source Gaussian Plume)	Weaver and Charbeneau (1989, 1990); Charbeneau and Johnson (1990)	KOPT: 1-D, vertical OILENS: 2-D, radial TSGPLUME:2-D	Analytical or semianalytical method of characteristics (MOC)	KOPT: ***W, O***, *V* (diffusion) OILENS: ***W, O***, *V* (diffusion) TSGPLUME: ***W***	Porous; homogeneous, isotropic Unsaturated	2-component LNAPL: (1) soluble and sorbing, (2) contaminant of interest partitions between *W, O, V*, and *S*. No dispersion	Linear, equilibrium, *W-O-V* partitioning. KOPT and OILENS for LNAPL intrusion through vadose and lateral (radial) spread at the water table w/ dissolution, volatilization from vadose and top of lens. TSGPLUME for solute dispersal w/ 1-order decay	Set of simple models for screening analysis. KOPT based on kinematic wave theory. KOPT/OILENS simulate oil dispersal and aqueous solute flux to groundwater; TSGPLUME simulates groundwater transport
MAGNAS (Multiphase Analysis of Groundwater, NAPL, And Soluble components)	Huyakorn, Panday, and Wu (1992); HydroGeoLogic, Inc.	3-D	FEM; linear rectangular elements	***W***, ***O*** (L or DNAPL), ***V***	Porous, heterogeneous, anisotropic	1	Equilibrium partitioning (*W-O-V-S*), first-order degradation	Proprietary code. Uses an enhanced influence-coefficient algorithm

(Sheet 1 of 5)

[1] Phases: *W* = water, *O* = organic liquid, *V* = vapor; *S* = solid; Advected phase symbols in ***bold italics***.
[2] Comments: VG = van Genuchten S-P_c model.; B-C = Brooks-Corey S-P_c model; NC = negligible capillarity (sharp interface). *Research* codes are those developed for process elucidation and have minimal distribution or support or application (validation); source codes may or may not be available. *Public domain* codes are those for which the source codes can be obtained at negligible cost. *Proprietary* codes are those for which source codes are not available.

Table A6 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Phases	Matrix Properties	Number of Components	Transport Processes Treated	Comments
MOTRANS	Envir. Syst. and Tech. (1991)	2-D, planar or radially sym. (vert.)	FEM; Adaptive Solution Domain	*W*, *O*, *V*	Porous; heterogeneous	5, noninteracting	*W-O-V-S* partitioning; equilibrium or 1st-order kinetics	Proprietary version of MOFAT; reportedly "improved efficiency, accuracy and robustness"; Preprocessor and postprocessor; VG or B-C
MOFAT	Katyal, Kaluarachchi and Parker (1991); ES&T							Public domain code developed for EPA (source code from Kerr Lab). VG only
MPNEG (Multi-Process Non-Equilibrium transport by Gas advection)	Brusseau (1991)	1-D	FD	*W*, *V*	Porous, structured	1	Nonequilibrium (1st-order) mass transfer between residual *W* and *V*; sorption from *W* only	Research code for evaluating effects of multiple non-equilibrium processes on gas advective transport
MPNEOIL (MPNE with Organic Immiscible Liquid)	Brusseau (1992)			*W*, *O*			Nonequilibrium mass transfer from *O* in mobile or immobile water zones, *W-O* mass transfer w/wo intra-NAPL diffusion	Research code to simulate the effects of non-equilibrium processes on NAPL distribution. Limited testing of MPNE models

(Sheet 2 of 5)

Table A6 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Phases	Matrix Properties	Number of Components	Transport Processes Treated	Comments
ULTRA (SESOIL+SUTRA)	Tucker, Huang, Bral, Dickinson (1986)	SESOIL: 1-D, vertical SUTRA: 2-D, areal	FD compartment FEM	*W*, *O* (residual), *V* (volatilization, at water table)	Porous	1	*W-O-V* equilibrium; leaching of residual NAPL by infiltrating rainwater or water table fluctuation; adsorption; biodegradation (0th order at high *C*; 1st order at low *C*)	Field tested; organic source depletion considered
UTCHEM	Datta Gupta et al. (1986); Saad, Pope, and Sepehrnoori (1989)	3-D	FD, 3rd-order	*W*, *O*, *V*	Porous, heterogeneous, anisotropic	Up to 19	Equilibrium (or non-) partitioning by pseudophase theory and hand equations. Adsorption. Surfactants effects	Compositional simulator developed for petroleum reservoir EOR by surfactant, micellar, cosolvent, or polymer flooding. Isothermal
STMVOC	Falta et al. (1992a,b)	3-D	IFD	*W*, *O*, *V*	Porous or fractured, heterogeneous, anisotropic	1 solute, heat	Equilibrium partitioning between *W*, *O*, *V*, and *S* phases	Developed from MULKOM (or TOUGH; see fractured media models) to simulate steam injection for NAPL recovery
2D-DIFF	Silka (1986)	2-D, areal	FD	*W* (immobile) *O* (residual) *V* (diffusion)	Porous; homogeneous, isotropic	1	*W/O-V* equilibrium	Designed for soil gas survey interpretation; developed by Hydrosystems, Inc.

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Table A6 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Phases	Matrix Properties	Number of Components	Transport Processes Treated	Comments
None	Abriola (1983, 1984); Abriola and Pinder (1985); Pinder and Abriola (1986)	2-D, vertical; (A&P (1985) are 1-D)	FD	*W*, *O*, *V* (diffusion)	Porous; heterogeneous, anisotropic; compressible	2: one volatile, one nonvolatile and nonreactive	*W-O-V* equilibrium of 1 component; compressible matrix and liquid	*VG*; coupled flow and transport; composition-dependent density and viscosity
None	Allan , R. E. (1986) M.S.-Waterloo	2-D (vertical)	FEM	*W* *O* (residual) *V* (adv. and diffus.)	Porous	1	*W-O-V* equilibrium. No reactions	Research code
None	Baehr (1987) USGS (NJ)	2-D, radial (r-z)	FD	*W* (constant, vertical flux), *O* (residual), *V* (diffusion)	Porous; homogeneous, isothermal	Multicomponent NAPL	Nonreactive	Research code. Air phase at atmospheric pressure
None	Baehr and Corapcioglu (1987); Corapcioglu and Baehr (1987)	1-D, vertical	FD	*W*, *O* (residual), *V* (diffusion)	Porous; homogeneous; unsaturated (constant)	Multicomponent NAPL	*W-O-V* equilibrium; adsorption (linear); oxygen-limited biodegradation	Research code. Partitioning is function of activity coefficients
None	Forsyth (1988)	2-D, vertical	FD	*W* (no dispersion), *O*, *V* (diffusion)	Porous, heterogeneous	1	*W-O-V* equilibrium	Research code
None	Fried, Munster, and Zillox (1979)	1-D	AN	*W*, *O* (floating lens)	Porous, homogeneous, isotropic. Saturated	1	*W-O* equilibrium	Sharp-interface NAPL lens modeled as point source. Water flow through residual NAPL zone
None	Mendoza and Frind (1990a,b)	2-D, vertical or axisymmetric	FEM	*W*, *O*, *V* (adv., diff.)	Porous	1	*W-O-V* equilibrium	Research code for developed for vapor extraction of residual NAPLs. B-C

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Table A6 (Continued)

Model Name	Authors	Dimensions	Solution Technique	Phases	Matrix Properties	Number of Components	Transport Processes Treated	Comments
None	Hoffmann (1969, 1971)	1-D	AN	*W*, *O* (lens)	Porous; homogeneous, isotropic	1	*W-O* equilibrium	Sharp-interface NAPL lens as point-source boundary (constant source). Water flow parallel to lens-water interface
None	Silka (1986)	2-D vertical	FD	*W*, *O* (residual), *V*	Porous	1	*W-O-V* equilibrium	Research code

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Table A7
Multiphase Flow Models

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Technique	Phases[1] (advected in bold)	Matrix/Fluid Properties	Supporting Documentation or Software	Availability	Comments
Numerical Models								
ARMOS	Kaluarachchi and Parker (1988) Environmental Sciences and Technology	2-D areal	FE	**W**, **O**, **V**	Porous; heterogeneous	Preprocessor and postprocessor; user's instructions with sample problems; SURFER-compatible output	$950 (750 nodes), $2,995 (2,500 nodes), $5,495 (7,500 nodes) from Scientific Software Group	van Genuchten constitutive eqns; LNAPLs only, PC version; executable only
FAMOS	Pawha INTERA Technologies	3-D	FD	**W**, O, V (2 at a time)	Porous; fractured; heterogeneous; compressible	In-house user's instructions	Proprietary	Compressible fluids
FDIM	Arthur D. Little, Inc. (1983)	1-D	FD	**W**, **O**	Porous; heterogeneous; saturated; incompressible	No complete documentation of the code exists	Unknown	Incompressible fluids; hysteretic P_c-S curve
IFLOW	Kuppasamy et al. (1987) Virginia Tech	2-D vertical	FE	**W**, **O**, **V** (atmos.)	Porous; heterogeneous; anisotropic	User's instructions with sample problems	Public domain	PC based; van Genuchten constitutive eqns
OILSPL	Lujan (1985) Colorado State University	1-D	FE	**W**, O, V	Porous; homogeneous; isotropic; incompressible	No user's instructions; unsupported	Unknown	Incompressible flow

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[1] Phases: W = water, O = oil or organic liquid, V = vapor; SW = salt water (represented as a separate phase).

Table A7 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Technique	Phases1 (advected in bold)	Matrix/Fluid Properties	Supporting Documentation or Software	Availability	Comments
Numerical Models (Concluded)								
SWANFLOW	Faust (1985) GeoTrans, Inc.	3-D	FD	**W**, **O**, V (atmos.)	Porous; heterogeneous; anisotropic; saturated/ unsaturated	User's instructions with sample problems; preprocessor and postprocessor	V. 3.3 is $700 plus $800 annual maintenance or $500 unsupported at GeoTrans; V. 1.0 is $120 at IGWMC with source code	Fluids are incompressible; air is at atmospheric pressure
WSTIF	Osborne and Sykes (1986) University of Waterloo	2-D vertical	FE	**W**, **O**	Porous; heterogeneous; anisotropic; saturated	No user's instructions; limited support	Unknown	Applied to Hyde Park landfill
None	Forsyth (1988) University of Waterloo	2-D	FD	**W**, **O**, V (atmos.)	Porous; heterogeneous; saturated/ unsaturated	Unknown	Unknown	Uses variable substitution to preclude the assignment of small nonwetting phase saturations
None	Hochmuth and Sunada (1985) Colorado State University	2-D areal	FE	**W**, **O**, **V** (2 at a time)	Porous; heterogeneous; unconfined	No user's instructions; unsupported	Unknown	
None	University of Waterloo	2-D vertical	FD	**W**, **O**	Porous; heterogeneous; anisotropic	No user's instructions; described in journal articles	Unknown	Recast two-phase equations to solve for wetting phase pressure and saturation; examines heterogeneities; Brooks-Corey constitutive equations

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Table A7 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimensions	Solution Technique	Phases1 (advected in bold)	Matrix/Fluid Properties	Supporting Documentation or Software	Availability	Comments
Analytical and Semianalytical Models								
KOPT	Weaver and Charbeneau (1989) University of Texas	1-D	Semi-analytical/ Method of characteristics (MOC)	**W, O**	Porous; homogeneous; isotropic; unsaturated	Preprocessor and postprocessor and sample problems	Public domain	
MOTOGRO	van der Veer (1979) Rijkswaterstaat, The Hague	2-D vertical	Semi-analytical	**W, O**	Porous; heterogeneous; anisotropic; confined/ unconfined	User's instructions with sample problems; no preprocessor or postprocessor	Unknown	Uses analytical function method
Modified MOC	Corapcioglu and Hossain (1986) Texas A&M University	2-D	Semi-analytical/ MOC	**W, O**	Porous; homogeneous; isotropic; unconfined saturated	Unknown	Unknown	Assumes constant flow rate; simulates lateral spreading
None	Illangasekare and Reible (1987) University of Colorado	1-D	Semi-analytical	**W, O**	Porous; homogeneous; isotropic; unsaturated	Limited documentation	Public domain	Assumes residual, immobile water
None	Colorado State University	1-D	Semi-analytical	**W, O**	Porous; homogeneous; saturated, incompressible	Unknown	Public domain	Limited boundary conditions, includes capillarity
Saltwater/Freshwater Models								
INTERFACE	Page (1979) Princeton University	2-D	FE	**W** SW	Porous; heterogeneous; isotropic; confined/ unconfined	User's instructions with sample problems	Unknown	
SEAWTR/ SEACONF	Allayla (1980) Colorado State University	2-D	FD	**W, SW**	Porous; heterogeneous; anisotropic; confined/ unconfined	User's instructions with sample problems	Unknown	Includes capillary effects

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Table A7 (Continued)

Model Name	Author or Contact and Institution (with reference if known)	Dimen-sions	Solution Technique	Phases1 (advected in bold)	Matrix/Fluid Properties	Supporting Documentation or Software	Availability	Comments
Saltwater/Freshwater Models (Continued)								
SHARP	Essaid (1990) USGS	2-D, quasi 3-D	FD	**W,** SW	Porous; heterogeneous; anisotropic; confined/ unconfined/ semiconfined	User's instructions with sample problems	Public domain	
SSIM3D		3-D	FD	**W,** SW			Public domain	
SWIFT		2-D vertical	FE	**W,** SW			Unknown	
SWIGS2D		2-D areal	FE	**W,** SW			Unknown	
SWSOR		2-D areal	FD	**W,** SW			Unknown	
3DSALT	Yeh et al. (1994)	3-D	FE flow FE-LE transport	**W,** SW	Porous; heterogeneous; anisotropic	User's manual comprehensive graphical user environment (GMS)	Public domain (code)	Coupled 3DFEMWATER and 3DLEWASTE

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Appendix B: Equilibrium Partition Formulations

Equilibrium Sorption

Sorption refers to any interaction between a solute and a solid. This intentionally broad definition includes strictly physical processes such as absorption as well as site-specific, chemical interactions such as ion exchange. Equilibrium sorption refers to the steady-state condition in which the rate of adsorption (mass transfer to the solid) equals the reverse process, desorption.

The local equilibrium assumption (LEA) is one of the most commonly made assumptions in modeling contaminant transport in the subsurface. The LEA is based on at least two assumptions: (a) that sorption kinetics are rapid relative to advective transport, and (b) the solute contacts all solid surfaces equally. Since groundwater moves relatively slowly, at least under low, natural gradients, the first assumption of chemical equilibrium where solute and solid meet is reasonable as a first approximation and often is valid. The second assumption is one of physical equilibrium and is never strictly true, particularly in strongly heterogeneous systems, but is a useful initial approximation without which an impractical level of media characterization is required. Physical heterogeneities, so common in the subsurface, can introduce a diffusion-limited, transport process between relatively high advection zones (e.g., coarse sands or fractures) and low advection zones (e.g., silt-clay lenses or crystalline matrix). This physical nonequilibrium is particularly important in aquifer decontamination, where solutes have had long residence times during which to penetrate low mobility zones such as silt or clay lenses. The transport resistance induced by physical heterogeneities is difficult both to overcome and to even describe predictively, and is currently an active area in contaminant transport research.

Sorption Isotherms

Solute transport codes employ a variety of mathematical descriptors for sorption. The traditional approach to describing equilibrium sorption is the isotherm, a mathematical expression or model of the dependence of

sorbate concentration on sorbent or solute concentration. The ratio of sorbate to solute concentration is the partitioning or distribution coefficient, K_d, which is the "local" slope of the isotherm equation. The three most commonly employed equilibrium partitioning models are as follows (see Figure B1):

- Linear partitioning $S = K_d C$ (B1a)
- Freundlich isotherm $S = K_F C^n$ (B1b)
- Langmuir isotherm $S = K_L S_{max} C/(1 + K_L C)$ (B1c)

where S is the sorbate or solvent concentration (mass sorbate per mass sorbent) and C is sorbent or solute concentration ($M\ L_{sol}^{-3}$). K_d, K_F, K_L, n, and S_{max} are, in practice, empirically determined or fitted parameters though they have conceptual or chemical basis. For example, the S_{max} represents the finite sorptive capacity of a sorbent, an appropriate concept for site-specific interactions such as ion exchange.

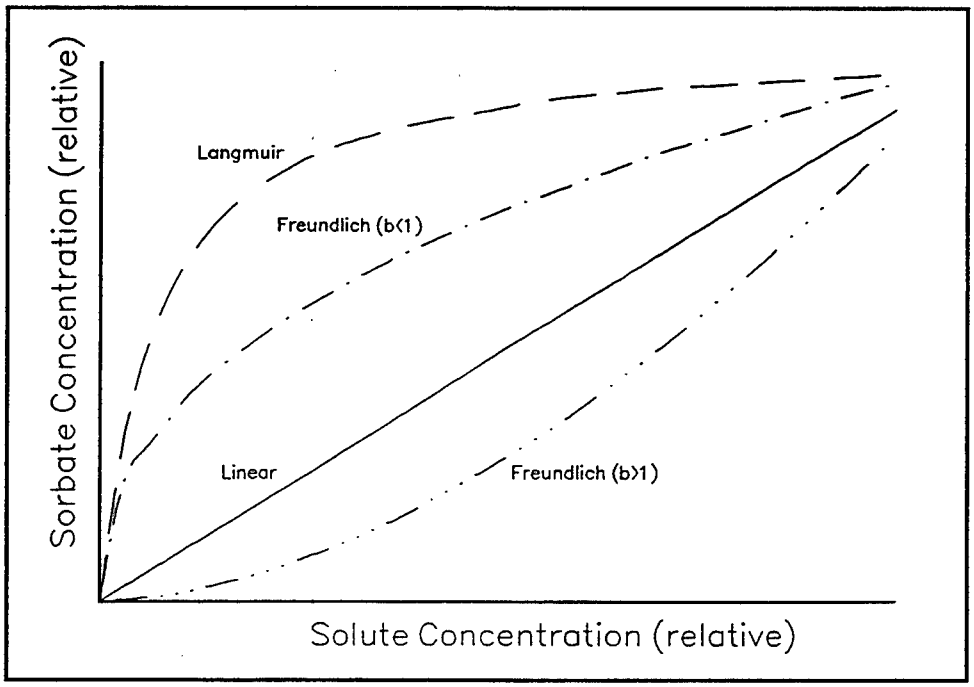

Figure B1. Schematic of common isotherms: Linear, Langmuir, and Freundlich with $b < 1$ and $b > 1$. K_d is the isotherm slope

The linear partitioning model is applicable when the ratio of solute i concentration in water ($M_i\ L^{-3}$) to solvent or sorbate i concentration ($M_i\ M_{sorbent}$) is constant over the concentration range of observation. A linear model is often acceptable over limited ranges of solute concentration. For example, nonpolar, hydrophobic organic solutes commonly partition in a nearly linear fashion at low concentration ranges, even though the isotherm may become nonlinear at higher concentrations. Munz and Roberts (1986) suggest that nonpolar, organic solutes typically show a linear partitioning behavior below 0.003 mole fraction (or 0.056 M). Karickhoff (1981) suggests that isotherms are likely to be linear for concentrations

below 0.003 molar and half of the solute's solubility limit. These rules-of-thumb strictly should not be extended to nonpolar, ionizable or ionic species, which if they adsorb significantly, involve specific sorption interactions, i.e., may be sensitive to multiple sorbent site populations, competitive sorption, or other complicating phenomena. The sorption mechanism for nonpolar, hydrophobic organics is a simpler, nonsite-specific, hydrophobic partitioning mechanism.

The Freundlich and Langmuir models are two of the most commonly utilized nonlinear isotherms. The nonlinearity reflects the varying capacity of the sorbent(s) to adsorb solute as the solute concentration varies. Commonly the sorptive capacity for a given substrate is finite; so as the sorption sites or surfaces are filled, a lesser proportion of the solute can be removed from solution. Thus, the "local" partitioning coefficient (slope of S versus C) tends to decrease with increasing C.

The Langmuir isotherm shows a clear limit to the sorptive capacity of the sorbent (S_{max}), as shown in Figure B1. The Freundlich isotherm may show a trend superficially similar to the Langmuir when the b_F is less than one (the typical case), though the model imposes no limit to sorptive capacity. If the b_F is greater than 1, the sorptive capacity theoretically approaches infinity, though solubility limits preclude this.

Multiple isotherm models can be utilized to describe sorption behaviors where multiple solute-sorbent interactions occur due to multiple sorbents, sorbates, or both. Few codes attempt such complexity.

Ion Exchange

All sorption reactions that involve specific interactions between ionic or strongly polar, solute molecules or functional groups and sorbent sites necessarily involve the exchange of solutes. The sorption mechanism for polar or ionic substances commonly involves a charge imbalance in the sorbent that is satisfied by a solute ion or partially satisfied by the polar nature of the sorbent molecule or functional group. Electroneutrality demands that a charge balance be maintained at all times. Thus, adsorption of a new solute, e.g., a contaminant, necessarily involves the desorption of a preexisting counterion. The exchange reaction may be described as:

$$m\,C_1^{n} + n\,S_2 \;\Leftrightarrow\; m\,S_1 + Nc_2^{m} \qquad \textit{(Rxn 1)}$$

where

n and m = valences of ions *1* and *2*, respectively

C = solute concentration

S = sorbent concentration

When the adsorption of the solute of concern is not affected appreciably by the displaced solute concentration, simple isotherms may be adequate to describe the process. If there is concentration-dependent competition

between the solute of interest and the pre-existing sorbate for sorption sites, then an ion exchange model is required.

Assuming equilibrium for Reaction 1, an ion selectivity coefficient may be defined (Freeze and Cherry 1979):

$$K_m = \frac{(S_1)^m (C_2)^n}{(S_2)^n (C_1)^m} \tag{B2}$$

where the parentheses indicate concentration in moles or equivalents per volume of solution or sorbent.

Assuming that the total solution concentration (in equivalents) and the ion exchange capacity (X, $M_{(eqv)} \cdot M^{-1}$) are constant, concentrations of the displacing ion-2 can be defined in terms of ion-1 (Grove and Stollenwerk 1984):

$$C_2 = (C_0 - nC_1) / m \tag{B3a}$$
$$S_2 = (X - nS_1) / m \tag{B3b}$$

where C_0 is the total solute concentration ($M_{equiv} L^{-3}$), which is constant in terms of equivalents. These expressions may be substituted into Equation B2 for a selectivity coefficient for solute-2 in terms of only solute-1:

$$K_m = \frac{S_1^m \left(\frac{C_0 - nC_1}{m}\right)^n}{C_1^m \left(\frac{X - nS_1}{m}\right)^n} \tag{B4}$$

Equation B4 can be rearranged to express S in terms of the other parameters. Then, $\partial S/\partial C$ can be determined and substituted into Equation B7 to define retardation factors (see next section).

Retardation Factors

The net effect of reversible sorption is to impede or retard the advance of the solute plume, and at the other end of the spectrum, to prolong a lower level of contamination over time. A simple approach to capturing this phenomena in a solute transport model is to introduce a coefficient to the advection-dispersion transport equation, the effect of which is to reduce solute "velocity" relative to the velocity of the associated water parcel. A simple, one-dimensional form of the advection-dispersion equation is:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} - \frac{\rho_b}{n_e} \frac{\partial S}{\partial t} \tag{B5}$$

The last term describes the influence of sorption on solute transport, which may be expanded (chain rule) to:

$$\frac{dS}{dt} = \frac{dS}{dC}\frac{\partial C}{\partial t} \tag{B6}$$

Substituting Equation B6 into B5 and rearranging yields:

$$\frac{\partial C}{\partial t}\left[1 + \frac{\rho_b}{\varepsilon}\frac{\partial S}{\partial C}\right] = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} \tag{B7}$$

The bracketed term is called the retardation factor. Of course, the $\partial S/\partial C$ term in the brackets is the sorption isotherm. Thus, retardation factors can be developed from any of the isotherm models (Equations B1a-B1c) as well as for ion exchange (B4).

This retardation factor (R_f) concept is probably the most commonly utilized approach to describe nonconservative solute behavior in numerical, transport codes, e.g., USGS-MOC, MT3D, and analytical solutions. The implicit assumptions made when evoking the retardation factor approach are that:

- Equilibrium partitioning is established instantaneously, or at least rapidly relative to the advective transport.
- No other reactions compete for the solute(s) of interest.
- Conditions are isothermal.

For linear partitioning (Equation B1a), the retardation factor is simply:

$$R_f = 1 + \frac{\rho_b K_d}{\varepsilon} \tag{B8}$$

where

ρ_b = bulk density of medium (typically 1.1 to 2.0 g cm^{-3})

ε = effective porosity (typically 0.20 to 0.35 for unconsolidated sand

The retardation factor based on the Freundlich isotherm also is derived quite simply by substituting the $\partial S/\partial C$ of Equation B1b into the advection-dispersion Equation B7 to yield:

$$R_f = 1 + \frac{\rho_b}{\varepsilon} n K_f C^{(n-1)} \tag{B9}$$

The Langmuir isotherm retardation factor is similarly derived to yield:

$$R_f = 1 + \frac{\rho_b}{\varepsilon}\frac{K_L S_{max}}{(1 + K_L C)^2} \tag{B10}$$

Retardation factors for simple ion exchange reactions (dual solute, single-site) are more complex since the descriptor depends on the ion valences and selectivity coefficients as well as concentrations. The sorption isotherm for ion-2 will be a function of ion-1 concentrations, ion valences m and n, C_0 , K_m , and X. Grove and Stollenwerk (1984) developed several linearized retardation factors for the four possible ion exchange cases: (a) monovalent displacing monovalent, (b) divalent displacing divalent, (c) monovalent displacing divalent, and (d) monovalent displacing divalent. For the monovalent-monovalent case (e.g., Na^+ displacing K^+):

$$R_{f(Na)} = 1 + \frac{\rho_b}{\varepsilon} \frac{K_m X C_0}{\left[C(K_m - 1) + C_0\right]^2} \tag{B11}$$

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13. ABSTRACT *(Maximum 200 words)*

The U.S. Army Engineer Waterways Experiment Station Groundwater Modeling Team performed a broad review of available groundwater models and an assessment of Army modeling. The first step was a model screening based primarily on current and anticipated Army and Department of Defense needs, followed by a more rigorous evaluation. This report provides the initial evaluation of more than 12 groundwater models that were selected based on the screening criteria. The effort included scrutiny of the code structure, certain process formulation, and performance evaluation relative to appropriate problems for which analytical solutions are available and/or hypothetical scenarios.

Four classes of models were evaluated: (1) saturated flow and/or transport, (2) coupled unsaturate/saturated flow and/or transport, (3) unsaturated flow and/or transport, and (4) multiphase models. Model performance in the initial evaluation was acceptable for the suite of models.

The second step was to evaluate/compare the models against analytic solutions, hypothetical scenarios, and/or filed data. Class (1) models were evaluated against analytic solutions for a line and point source in a homogeneous aquifer and against a hypothetical scenario. Results were adequate, although several models exhibit some discrepancies against the analytical

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solution. Class (2) models were evaluated against field data from a two-dimensional infiltration experiment. Simulation results were mixed; some models were able to simulate the behavior from the experimental data, while others were only able to simulate the pattern, but not the full behavior. The results show that models or descriptors for pressure/saturation and hydraulic conductivity/saturation curves are very important in simulating unsaturated/ saturated flow. Class (3) and (4) models were only evaluated against the example problems since a complete data set for either class was extremely hard to find.